Towards first-principle description of electromagnetic reactions in medium-mass nuclei

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Motivations

Electromagnetic probes (coupling constant $<<1$)

"With the electro-magnetic probe, we can immediately relate the cross section to the transition matrix element of the current operator, thus to the structure of the target itself"

[De Forest-Walecka, Ann. Phys. 1966]

$$\sigma \propto \left| \langle \Psi_f \mid J^\mu \mid \Psi_0 \rangle \right|^2$$
Motivations

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- For few-nucleons one can perform exact calculations both for bound and scattering states test the nuclear theory on light nuclei and extend it to heavier mass number
Motivations

- Electromagnetic probes (coupling constant <<1)

"With the electro-magnetic probe, we can immediately relate the cross section to the transition matrix element of the current operator, thus to the structure of the target itself"

\[ \sigma \propto \left| \langle \Psi_f | J^\mu | \Psi_0 \rangle \right|^2 \]

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- For few-nucleons one can perform exact calculations both for bound and scattering states to test the nuclear theory on light nuclei and extend it to heavier mass number

- Provide important informations in other fields of physics, where nuclear physics plays a crucial role:
  - Astrophysics: $\gamma$ interactions with nucleonic matter, radiative capture reactions, $\nu$ interactions with nucleonic matter (vector current as em)
  - Atomic physics (nuclear corrections to atomic levels, etc.)
  - Particle physics (neutrino-interaction with nuclei)
Electromagnetic Reactions

- Photonuclear Reactions
- Electric-Dipole Polarizability
Reactions resulting from the interaction of a photon with the nucleus

For photon energy 15-25 MeV stable nuclei across the periodic table show a wide and large peak
Photo-nuclear Reactions

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*Ahrens et al.*

Giant Dipole Resonance
Photo-nuclear Reactions

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Coulomb excitations

Inelastic scattering between two charged particles. Can use unstable nuclei as projectiles.

Neutron-rich nuclei show fragmented low-lying strength

Giant Dipole Resonance

Leistenschneider et al.
Photo-nuclear Reactions

Reactions resulting from the interaction of a photon with the nucleus

For photon energy 15-25 MeV stable nuclei across the periodic table show a wide and large peak

Can we give a microscopic explanation of these observations?

Coulomb excitations

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Neutron-rich nuclei show fragmented low-lying strength

Leistenschneider et al.
High precision two-nucleon potentials: well constraint on NN phase shifts

Three nucleon forces: less known, constraint on A>2 observables
Ab-initio Theory Tools

High precision two-nucleon potentials: well constraint on NN phase shifts

Three nucleon forces: less known, constraint on A>2 observables

$H |\psi_i\rangle = E_i |\psi_i\rangle$

$H = T + V_{NN} + V_{3N} + ...$

two-body currents (or MEC) subnuclear d.o.f.

$J^{\mu} = J^{\mu}_N + J^{\mu}_{NN} + ...$

$\nabla \cdot J = -i[V, \rho]$
**Ab-initio Theory Tools**

\[ H \psi_i = E_i \psi_i \]

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- High precision two-nucleon potentials: well constraint on NN phase shifts
- Three nucleon forces: less known, constraint on A>2 observables

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Two-body currents (or MEC) subnuclear d.o.f.

\[ \nabla \cdot J = -i[V, \rho] \]

Traditional Nuclear Physics
- AV18+UIX, ..., \( J_2 \)

Effective Field Theory
- \( N^2\text{LO}, N^3\text{LO} \ldots \)
High precision two-nucleon potentials: well constraint on NN phase shifts

Three nucleon forces: less known, constraint on A>2 observables

\[ H |\psi_i\rangle = E_i |\psi_i\rangle \]

\[ H = T + V_{NN} + V_{3N} + \ldots \]

\[ J^\mu = J_N^\mu + J_{NN}^\mu + \ldots \]

two-body currents (or MEC) subnuclear d.o.f.

\[ J^\mu \text{ consistent with } V \]

\[ \nabla \cdot J = -i[V, \rho] \]

\[ \sigma \propto \left| \langle \Psi_f | J^\mu | \Psi_0 \rangle \right|^2 \]

Exact Initial state & Final state in the continuum at different energies and for different A
Lorentz Integral Transform Method


Reduce the continuum problem to a bound-state problem

\[ R(\omega) = \sum_f \left| \langle \psi_f | J^\mu | \psi_0 \rangle \right|^2 \delta(E_f - E_0 - \omega) \]

\[ L(\sigma, \Gamma) = \int d\omega \frac{R(\omega)}{(\omega - \sigma)^2 + \Gamma^2} = \left\langle \tilde{\psi} | \tilde{\psi} \right\rangle < \infty \]

where \( |\tilde{\psi}\rangle \) is obtained solving

\[ (\mathcal{H} - E_0 - \sigma + i\Gamma) |\tilde{\Psi}\rangle = J^\mu |\Psi_0\rangle \]

- Due to imaginary part \( \Gamma \) the solution \( |\tilde{\psi}\rangle \) is unique
- Since \( \left\langle \tilde{\psi} | \tilde{\psi} \right\rangle \) is finite, \( |\psi\rangle \) has bound state asymptotic behaviour

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Lorentz Integral Transform Method


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\[ L(\sigma, \Gamma) \xrightarrow{\text{inversion}} R(\omega) \]

The exact final state interaction is included in the continuum rigorously!
Lorentz Integral Transform Method


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Solved for \( A=3,4,6,7 \) with hyper-spherical harmonics expansions and for \( A=4 \) with NCSM

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Photoabsorption of A=6 with Hyperspherical Harmonics

\[ \sigma_\gamma = \frac{4\pi^2\alpha}{3} \omega R^{E1}(\omega) \]

\[ E1 = \sum_{i=1}^{Z}(z_i - Z_{cm}) \]

\[ T_{1/2} = 806 \text{ ms} \]

No cluster assumption was used in this calculation. Potential: AV4'.
Hyperspherical Harmonics
A basis set, mostly used for $A=3,4$. Challenge to go up to $A=7,8$

\[
\Psi = \sum_{[K],\nu} c_{\nu}[K] e^{-\rho/2} \rho^{n/2} L_{\nu}^n(\rho) [\mathcal{Y}_K(\Omega)]^{\mu}_{\nu} \chi_{ST}^{\mu} J_T
\]

Ground States

For the reactions expanding

\[
(H - E_0 - \sigma + i\Gamma)|\tilde{\Psi}\rangle = J^{\mu} |\Psi_0\rangle
\]

increase of dimension by at least one order of magnitude if angular momentum is changed.
Hyperspherical Harmonics

A basis set, mostly used for \( A=3,4 \). Challenge to go up to \( A=7,8 \)

\[ \Psi = \sum_{[K], \nu} c^K_{\nu} e^{-\rho/\nu} \rho^{\nu/2} L^{n}_{\nu}(\rho) [Y^{\mu}_{[K]}(\Omega) \chi^{\mu}_{ST}]^{\alpha}_{\beta} \]

For the reactions expanding, increase of dimension by at least one order of magnitude if angular momentum is changed.

\[ (H - E_0 - \sigma + i \Gamma) |\Psi\rangle = J^\mu |\Psi\rangle \]

Total number of states: 
\( \#HH \times \#\text{Hyper-radial states} \)

\( 10^6 \) dense matrix
Develop new many-body methods that can extend the frontiers to heavier and neutron nuclei

- CC is optimal for closed shell nuclei ($\pm 1, \pm 2$)

Uses particle coordinates

$$|\psi_0(\vec{r}_1, \vec{r}_2, ..., \vec{r}_A)\rangle = e^T |\phi_0(\vec{r}_1, \vec{r}_2, ..., \vec{r}_A)\rangle$$

Reference SD with any sp states

$$T = \sum T_{(A)}$$  cluster expansion

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

$$T_2 = \frac{1}{4} \sum_{ij,ab} t_{ij}^{ab} a_i^\dagger a_j^\dagger a_j a_i$$  ...

$$T_1 \quad T_2 \quad T_3$$

CCSD Computational scaling  $n_o^2 n_u^4$

Coupled Cluster Theory
Extension to medium-mass nuclei

Develop new many-body methods that can extend the frontiers to heavier and neutron nuclei

Coupled Cluster Theory

- CC is optimal for closed shell nuclei ($\pm 1, \pm 2$)
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  reference SD with any sp states

\[ T = \sum T_{(A)} \quad \text{cluster expansion} \]

CC is a very mature theory for g.s., see e.g.


experiment

S. Binder et al, arXiv:1312.5685
Extension to medium-mass nuclei

Develop new many-body methods that can extend the frontiers to heavier and neutron nuclei

Coupled Cluster Theory

CC future aims

CC theory now

Coupled Cluster Theory

$T = \sum T(A)$ cluster expansion

CC is optimal for closed shell nuclei ($\pm 1, \pm 2$)

Uses particle coordinates

$|\psi_0(\vec{r}_1, \vec{r}_2, ..., \vec{r}_A)\rangle = e^T |\phi_0(\vec{r}_1, \vec{r}_2, ..., \vec{r}_A)\rangle$

reference SD with any sp states

$T = \sum T(A)$

CC is a very mature theory for g.s., see e.g.


What about electromagnetic reactions?

experiment

S. Binder et al, arXiv:1312.5685

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Wednesday, 25 June, 14
L(\sigma, \Gamma) = \int d\omega \frac{R(\omega)}{(\omega - \sigma)^2 + \Gamma^2} = \langle \tilde{\Psi} | \tilde{\Psi} \rangle

(H - z^*) | \tilde{\Psi} \rangle = J^\mu | \psi_0 \rangle

with \ z = E_0 + \sigma + i\Gamma
New theoretical method aimed at extending *ab-initio* calculations towards medium mass

\[
L(\sigma, \Gamma) = \int d\omega \frac{R(\omega)}{(\omega - \sigma)^2 + \Gamma^2} = \langle \tilde{\Psi} | \tilde{\Psi} \rangle
\]

\[
(H - z^*)|\tilde{\Psi}\rangle = J^\mu |\psi_0\rangle
\]

with \( z = E_0 + \sigma + i\Gamma \)

\[
(H - z^*)|\tilde{\Psi}_R\rangle = \tilde{\Theta} |\Phi_0\rangle
\]

\[
\tilde{H} = e^{-T} H e^T
\]

\[
\tilde{\Theta} = e^{-T} \Theta e^T
\]

EoM with source
New theoretical method aimed at extending \textit{ab-initio} calculations towards medium mass.

\[ L(\sigma, \Gamma) = \int d\omega \frac{R(\omega)}{(\omega - \sigma)^2 + \Gamma^2} = \langle \tilde{\Psi} | \tilde{\Psi} \rangle \rightarrow \langle \tilde{\Psi}_L | \tilde{\Psi}_R \rangle = \langle \Phi_0 \hat{L}(z) | \hat{R}(z^*) \Phi_0 \rangle \]

\[ (H - z^*)|\tilde{\Psi}\rangle = J^\mu |\psi_0\rangle \]

with \( z = E_0 + \sigma + i\Gamma \)

\[ \langle H - z^* \rangle |\tilde{\Psi}_R\rangle = \tilde{\Theta} |\Phi_0\rangle \]

\[ \tilde{H} = e^{-T} H e^T \]

\[ \tilde{\Theta} = e^{-T} \Theta e^T \]

\[ EoM \text{ with source} \]

EoM with source
L(σ, Γ) = \int d\omega \frac{R(\omega)}{(\omega - \sigma)^2 + \Gamma^2} = \langle \tilde{\Psi} | \tilde{\Psi} \rangle \rightarrow \langle \tilde{\Psi}_L | \tilde{\Psi}_R \rangle = \langle \Phi_0 \hat{L}(z) | \hat{R}(z^*) \Phi_0 \rangle

(H - z^*)|\tilde{\Psi}\rangle = J^\mu |\psi_0\rangle

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

(\hat{H} - z^*)|\tilde{\Psi}_R\rangle = \tilde{\Theta} |\Phi_0\rangle

\hat{H} = e^{-T}He^T
\tilde{\Theta} = e^{-T}\Theta e^T

In the CCSD scheme \ T = T_1 + T_2

\hat{R} = \hat{R}_0 + \sum_{ia} \hat{R}_{ia} \hat{c}_a ^\dagger \hat{c}_i + \frac{1}{4} \sum_{ijab} \hat{R}_{ijab} \hat{c}_a ^\dagger \hat{c}_b ^\dagger \hat{c}_j \hat{c}_i + \ldots

EoM with source
New theoretical method aimed at extending *ab-initio* calculations towards medium mass

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L(\sigma, \Gamma) = \int d\omega \frac{R(\omega)}{(\omega - \sigma)^2 + \Gamma^2} = \langle \tilde{\Psi} | \tilde{\Psi} \rangle \rightarrow \langle \tilde{\Psi}_L | \tilde{\Psi}_R \rangle = \langle \Phi_0 \hat{L}(z) | \hat{R}(z^*) \Phi_0 \rangle
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(H - z^*) | \tilde{\Psi} \rangle = J^\mu | \psi_0 \rangle
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with \( z = E_0 + \sigma + i\Gamma \)

\[
(H - z^*) \hat{R} | \Phi_0 \rangle = \tilde{\Theta} | \Phi_0 \rangle
\]

\[
\bar{H} = e^{-T} H e^T
\]

\[
\bar{\Theta} = e^{-T} \Theta e^T
\]

EoM with source

In the CCSD scheme

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\]

Validation for \(^4\text{He}\)

Dipole Response Functions

with NN forces from \(\chi\text{EFT (N}^3\text{LO)}\)
New theoretical method aimed at extending \textit{ab-initio} calculations towards medium mass

\textbf{Extension to Dipole Response Function in }^{16}\text{O with NN forces derived from }\chi\text{EFT (N}^3\text{LO)}

Convergence in the model space expansion

\begin{align*}
L & \text{[fm}^2\text{MeV}^{-2}10^{-2]} \\
\sigma & \text{[MeV]} \\
\Gamma & = 10 \text{ MeV} \\
N_{\text{max}} & \\
18 & \\
16 & \\
14 & \\
12 & \\
10 & \\
8 & \\
\hbar\Omega & = 26 \text{ MeV}
\end{align*}

Good convergence!
New theoretical method aimed at extending *ab initio* calculations towards medium mass

**Extension to Dipole Response Function in $^{16}$O with NN forces derived from $\chi$EFT (N$^3$LO)**

Convergence in the model space expansion

Good convergence!

Small HO dependence: use it as error bar
New theoretical method aimed at extending ab-initio calculations towards medium mass

Extension to Dipole Response Function in $^{16}$O with NN forces derived from $\chi$EFT (N$^3$LO)

Comparison to the experiment
New theoretical method aimed at extending *ab-initio* calculations towards medium mass.

**Extension to Dipole Response Function in $^{16}$O with NN forces derived from $\chi$EFT (N$^3$LO)**

Comparison to the experiment:

- LIT of data
- CCSD

Comparison to the experiment:

- Ahrens *et al.*
- Ishkanov *et al.*
- CCSD
New theoretical method aimed at extending *ab-initio* calculations towards medium mass.

**Extension to Dipole Response Function in $^{16}$O with NN forces derived from $\chi$EFT ($N^3$LO)**

Comparison to the experiment.

The GDR of $^{16}$O is described from first principles for the first time!
New theoretical method aimed at extending ab-initio calculations towards medium mass

Extension to Dipole Response Function in \(^{16}\text{O}\) with NN forces derived from \(\chi\text{EFT (N}^3\text{LO)}\)

Comparison to the experiment

\[
L = 10 \text{ MeV}
\]

\[
\Gamma = 10 \text{ MeV}
\]

The GDR of \(^{16}\text{O}\) is described from first principles for the first time!
Extension to Dipole Response Function in $^{22}\text{O}$ with NN forces derived from EFT (N$^3$LO)

Work in Progress

Convergence pattern similar to $^{16}\text{O}$
LIT with Coupled Cluster Theory

Extension to Dipole Response Function in $^{22}\text{O}$ with NN forces derived from EFT (N$^3$LO)

Work in Progress

Bremsstrahlung sum rule $\propto \left(\frac{NZ}{A}\right)^2 R_{PN}$

Convergence pattern similar to $^{16}\text{O}$
Extension to Dipole Response Function in $^{22}$O with NN forces derived from EFT (N$^3$LO)

LIT with Coupled Cluster Theory

Work in Progress

Bremsstrahlung sum rule $\propto \left( \frac{NZ}{A} \right)^2 R_{PN}$

Convergence pattern similar to $^{16}$O

The centroid of $^{22}$O seems ~ 3 MeV lower than for $^{16}$O
Theoretical GDR peaks are located at higher energies with respect to experiment: nuclei are over bound with smaller radii and thus one needs higher energy to excite the GDR.
Electric Dipole Polarizability
with NN(N^3LO)

\[ \alpha_E = \frac{1}{2\pi^2} \int_{\omega_{th}}^{\infty} d\omega \frac{\sigma_\gamma(\omega)}{\omega^2} \]

- calculated with the Lanczos algorithm

\( N_{\text{max}} \) vs. \( \alpha_E [\text{fm}^3] \) for \(^4\text{He}\)

\( h\Omega = 20 \text{ MeV} \)
\( h\Omega = 24 \text{ MeV} \)
\( h\Omega = 26 \text{ MeV} \)

\( N_{\text{max}} \) vs. \( \alpha_D [\text{fm}^3] \) for \(^{16}\text{O}\)

- EXPERIMENT

\( h\Omega = 20 \text{ MeV} \)
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LIT with Coupled Cluster Theory

with M. Miorelli

Electric Dipole Polarizability
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Towards an ab-initio theory for \(^{48}\text{Ca}\)

DFT prediction

\(^{48}\text{Ca}\) being measured at RCNP

\(^{48}\text{Ca} \quad \alpha_E \) being measured at RCNP
Electric Dipole Polarizability:

$$\alpha_E = \frac{1}{2\pi^2} \int_{\omega_{th}}^{\infty} d\omega \frac{\sigma_{\gamma}(\omega)}{\omega^2}$$

Energy Density Functional Theory (EDFT)


very correlated to the neutron-skin radius

Do we also see such a correlation with ab-initio methods?
Correlation of polarizability vs radius

\[ C_{AB} = 0.961 \]
Correlation of polarizability vs radius

\[ \alpha_E [\text{fm}^3] \]

\[ r_{\text{charge}} [\text{fm}] \]

\[ C_{AB} = 0.961 \]

Optimized $\chi$EFT interaction at $N^2$LO from Ekström et al.
Correlation of polarizability vs radius

- n2lo_opt_bare
- n2lo_opt38 (N=12)
- cdbonn_vlowk20
- cdbonn_vlowk25
- cdbonn_vlowk30
- cdbonn_srg35
- cdbonn_srg40
- n3lo500EM_srg20
- n3lo500EM_srg25
- n3lo500EM_srg30
- n3lo500EM_srg35
- n3lo600EM_srg20
- n3lo600EM_srg25
- n3lo600EM_srg30

+3NF

Optimized $\chi$EFT interaction at N$^2$LO from Ekström et al.

$C_{AB} = 0.989$
Correlation of polarizability vs skin-radius

$^{48}\text{Ca}$

DFT predictions

$\chiEFT$ interaction at $N^2$LO from Ekström et al.

$C_{AB} = 0.974$

$^{48}\text{Ca} \; \alpha_E$ being measured at RCNP

$^{48}\text{Ca}$ parity violating electron scattering at JLab, CREX
Electromagnetic break up reactions are very rich observables to test our understanding of nuclear forces.

Extending these calculations to medium mass nuclei is possible and very exciting, with hopefully more applications/impact on future experiments.
Conclusions and Outlook

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Perspectives

- Dipole response function of neutron-rich Oxygen isotope

- Other multipole excitation (quadrupole or monopole) of medium mass nuclei need extension to two-body operators

- Add triples and three-nucleon forces
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Thank you!