Electromagnetic strengths in ab-initio approaches

Sonia Bacca  |  TRIUMF

The 5th international conference on "COLLECTIVE MOTION IN NUCLEI UNDER EXTREME CONDITIONS"

Electromagnetic Reactions

Nuclear Halo

Pigmy Resonance

Tuesday, 15 September, 15
“Ab-initio” methods

- Start from neutrons and protons as building blocks (centre of mass coordinates, spins, isospins)

- Solve the non-relativistic quantum mechanical problem of $A$-interacting nucleons

$$H |\psi_i\rangle = E_i |\psi_i\rangle$$
$$H = T + V_{NN}(\Lambda) + V_{3N}(\Lambda) + \ldots$$

- Find numerical solutions with no approximations or controllable approximations (error bars)
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- Calculate low-energy observables and compare with experiment to test nuclear forces and provide predictions for future experiments or quantity that cannot be measured
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Dipole strength functions

Giant dipole resonance

Discrepancies

Narrow resonances

Continuum
Observables

Dipole strength functions

\[ \sigma_r [mb] \]

Continuum

Giant dipole resonance

Discreets levels

Narrow resonances

\[ \omega \text{ [MeV]} \]
Observables

Dipole strength functions

- Giant dipole resonance
- Narrow resonances
- Discrete levels

Pigmy dipole resonance in neutron-rich nuclei

ω [MeV]

σ_r [mb]

Continuum

8 16
Electric dipole polarizability
Electric dipole polarizability

\[ D = \alpha_D E \]

\[ \alpha_D = 2\alpha \int_{\omega_{th}}^{\infty} d\omega \frac{R_D(\omega)}{\omega} \]

Low-energy part of response dominates

Very interesting for neutron-rich nuclei:
soft modes at low energy enhance the polarizability
Stable Nuclei

We have data on ~180 stable nuclei
Giant dipole resonances

Unstable Nuclei

Fewer data, pigmy dipole resonances

From photoabsorption experiments

From Coulomb excitation experiments
Experimental status

Stable Nuclei

We have data on ~180 stable nuclei
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Unstable Nuclei

Fewer data, pigmy dipole resonances

From photoabsorption experiments

From Coulomb excitation experiments

Do we see the emergence of collective motions from first principle calculations?
48Ca - an interesting case

While neutron-rich, for all practical purposes it can be considered a stable nucleus

 Stellar (p,p') scattering to extract the electric dipole polarizability at RCNP, Japan

\( \alpha_D \) is related to the symmetry energy in the EOS of nuclear matter

 Parity violation electron scattering Calcium Radius Experiment (CREX) at JLab to measure \( R_{\text{skin}} \)

\[
A_{pv} = \frac{d\sigma/d\Omega_R - d\sigma/d\Omega_L}{d\sigma/d\Omega_R + d\sigma/d\Omega_L} \approx -\frac{G_F q^2}{4\pi\alpha\sqrt{2}} \frac{Q_W F_W(q^2)}{ZF_{ch}(q^2)}
\]

The weak force probes the neutron distribution

\( Q_W^n \approx -1 \)

\( Q_W^p = 1 - 4\sin^2\theta_W \approx 0 \)
While neutron-rich, for all practical purposes it can be considered a stable nucleus

\( \langle p,p' \rangle \) scattering to extract the electric dipole polarizability at RCNP, Japan

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The weak force probes the neutron distribution

\( Q^n_W \approx -1 \)

\( Q^p_W = 1 - 4\sin^2\theta_W \approx 0 \)

Can we give a first principle predictions for these future experiments?
These observables on medium and heavy nuclei have been the subject of intense theoretical studies within density functional theory, shell model, etc...

Not much has been done with ab-initio methods and we want to fill this gap!
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Not much has been done with ab-initio methods and we want to fill this gap!

*Electromagnetic Reactions on Light Nuclei*
*S. Bacca and S. Pastore*
\[ H |\psi_i\rangle = E_i |\psi_i\rangle \]

\[ H = T + V_{NN} + V_{3N} + \ldots \]
Ab-initio Approach

\[ H |\psi_i\rangle = E_i |\psi_i\rangle \]
\[ H = T + V_{NN} + V_{3N} + \ldots \]

\[ J^\mu = J^\mu_N + J^\mu_{NN} + \ldots \]

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

\[ J^\mu \text{ consistent with } V \]
\[ \nabla \cdot J = -i[V, \rho] \]
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\[ \nabla \cdot J = -i[V, \rho] \]
In the limit of vanishing quark masses the QCD Lagrangian is invariant under chiral symmetry.

Quark/gluon (high energy) dynamics

\[
\mathcal{L} = -\frac{1}{4} G_{\mu\nu}^{a} G_{a}^{\mu\nu} + \bar{q}_{L} i \gamma_{\mu} D^{\mu} q_{L} + \bar{q}_{R} i \gamma_{\mu} D^{\mu} q_{R} - \bar{q} M q
\]

In the limit of vanishing quark masses the QCD Lagrangian is invariant under chiral symmetry.

Chiral symmetry is explicit and spontaneous broken.
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Quark/gluon (high energy) dynamics

\[ \mathcal{L} = -\frac{1}{4} G^a_{\mu\nu} G^{a\mu\nu}_t + \bar{q}_L i \gamma_\mu D^\mu q_L + \bar{q}_R i \gamma_\mu D^\mu q_R - \bar{q} \mathcal{M} q \]

QCD chiral symmetry

Chiral symmetry is explicit and spontaneous broken.

Nucleon/pion (low energy) dynamics

\[ \mathcal{L}_{\text{eff}} = \mathcal{L}_{\pi\pi} + \mathcal{L}_{\pi N} + \mathcal{L}_{NN} + \ldots \]

Compatible with explicit and spontaneous chiral symmetry breaking.
### Chiral Effective Field Theory

**Systematic expansion**

\[ \mathcal{L} = \sum_{\nu} c_{\nu} \left( \frac{Q}{\Lambda_b} \right)^\nu \]

Details of short distance physics not resolved, but captured in **low energy constants (LEC)**

<table>
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<tr>
<th></th>
<th>2N force</th>
<th>3N force</th>
<th>4N force</th>
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<td>( \nu = 4 )</td>
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Chiral Effective Field Theory

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\[ \mathcal{L} = \sum_{\nu} c_{\nu} \left( \frac{Q}{\Lambda_b} \right)^{\nu} \]

Details of short distance physics not resolved, but captured in low energy constants (LEC)

LEC fit to experiment - NN sector -

Future: lattice QCD?
Now fit to experiment

Traditional Paradigm:
(i) Fit NN on scattering data first

Epelbaum et al. (2009)
Chiral Effective Field Theory

Systematic expansion
\[ \mathcal{L} = \sum_{\nu} c_{\nu} \left( \frac{Q}{\Lambda_b} \right)^\nu \]

Details of short distance physics not resolved, but captured in low energy constants (LEC)

LEC fit to experiment - NN sector -

\[ \nu = 0 \]
\[ \nu = 2 \]
\[ \nu = 3 \]
\[ \nu = 4 \]

Future: lattice QCD? Now fit to experiment

Traditional Paradigm:
(i) Fit NN on scattering data first
(ii) add 3N forces fitting on \(^3\text{H}/\(^3\text{He}\)

Epelbaum et al. (2009)
Ab-initio Approach

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

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

\[ J^\mu = J^\mu_N + J^\mu_{NN} + \ldots \]

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

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

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

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

Need many-body continuum effects
Lorentz Integral Transform Method


Reduce the continuum problem to a bound-state problem

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

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

where $|\tilde{\psi}\rangle$ is obtained solving

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

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

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

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


Reduce the continuum problem to a bound-state problem

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R(\omega) = \sum_f R_f^c \left| \left\langle \psi_f | J^\mu | \psi_0 \right\rangle \right|^2 \delta(E_f - E_0 - \omega)
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\[
L(\sigma, \Gamma) \overset{\text{inversion}}{\rightarrow} R(\omega)
\]

The exact final state interaction (FSI) is included in the continuum rigorously!

Solved for \(A=3,4,6,7\) with hyper-spherical harmonics expansions and for \(A=4\) with NCSM
Challenge: develop new ab-initio methods that can extend the frontiers to heavier nuclei

Coupled Cluster Theory

- Optimal for closed shell nuclei ($\pm 1, \pm 2$)

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

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

Very successful in nuclear theory

Extension to medium-mass nuclei

Challenge: develop new ab-initio methods that can extend the frontiers to heavier nuclei

Coupled Cluster Theory

CC future aims

CC theory now

Very successful in nuclear theory


Approximation schemes

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

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T_1, T_2, T_3
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Coupled Cluster Theory

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Approximation schemes

- Good computational scaling

Very successful in nuclear theory

Merging the Lorentz integral transform method with coupled-cluster theory: New many-body method to extend \textit{ab-initio} calculations of em reactions to medium-mass-nuclei

S.B. \textit{et al.}, PRL 111, 122502 (2013)

\[
\begin{align*}
\langle \bar{H} - z^* \rangle |\bar{\Psi}_R(z^*) \rangle &= \bar{\Theta} |\Phi_0 \rangle \\
\bar{H} &= e^{-T} H e^{T} \\
\bar{\Theta} &= e^{-T} \Theta e^{T}
\end{align*}
\]
Giant Dipole Resonances

Merging the Lorentz integral transform method with coupled-cluster theory:
New many-body method to extend ab-initio calculations of em reactions to medium-mass-nuclei

S.B. et al., PRL 111, 122502 (2013) → LIT-CCSD

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

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

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

Validation for $^4$He with exact hyperspherical harmonics

NN forces derived from chiral EFT (N$^3$LO)

The comparison is very good
Small difference due to missing triples and quadruples
Giant Dipole Resonances

Extension to heavier nuclei

NN forces derived from chiral EFT (N³LO)

S.B. et al., PRL 111, 122502 (2013)
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NN forces derived from chiral EFT (N^3LO)

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

The position of the GDR is described from first principles for the first time
Giant Dipole Resonances

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

S.B. et al., PRC 90, 064619 (2014)
Pigmy Dipole Resonances

Extension to neutron-rich nuclei

NN forces derived from chiral EFT (N$^3$LO)

S.B. et al., PRC 90, 064619 (2014)

With Mirko Miorelli, PhD student

$^{22}\text{O}$ data from GSI

C being measured at RIKEN

$^{22}\text{O}$

\[ \sigma(\omega) \text{ [mb]} \]

$^{22}\text{C}$

\[ \sigma(\omega) \text{ [mb]} \]

$S_n^{\text{exp}}$

Leistenschneider et al.

LIT-CCSD

LIT-CCSD

Preliminary
Pigmy Dipole Resonances

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S.B. et al., PRC 90, 064619 (2014)

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22O data from GSI

22C being measured at RIKEN

Soft dipole mode emerges from first principle calculations
Electric Dipole Polarizability

NN interactions

M. Miorelli et al., in preparation (2015)

\[ \alpha_D \, [\text{fm}^3] \]

16O

\[ R_{ch} \, [\text{fm}] \]

40Ca

\[ R_{ch} \, [\text{fm}] \]

NN only

NN only

\[ \text{exp} \]

\[ \text{NN only} \]
We observe correlations between polarizability and radii ($R_{ch}$, $R_p$, $R_n$)

**NN interactions**

M. Miorelli et al., in preparation (2015)
Electric Dipole Polarizability

NN interactions

M. Miorelli et al., in preparation (2015)

We observe correlations between polarizability and radii ($R_{ch}$, $R_p$, $R_n$)

Two-body Hamiltonian underestimates both radii and electric dipole polarizabilities
Including three-nucleon forces

We need accurate interactions able to reproduce both energies and radii.
Including three-nucleon forces

We need accurate interactions able to reproduce both energies and radii

\[ E/A \text{ (MeV)} \]

\[ \Delta r_{ch} \text{ (fm)} \]

\[
\begin{array}{cccc}
\text{He} & \text{He} & \text{C} & \text{O} & \text{Ca} \\
\end{array}
\]

Electric Dipole Polarizability

with 3N forces ★ $\text{NNLO}_{\text{sat}}$

---

**Graph 1:**
- $^{16}\text{O}$
- Plot of $\alpha_D$ vs. $R_{ch}$ in fm,
- Data points marked with different symbols and colors,
- $\alpha_D$ values on the y-axis from 0.2 to 0.6,
- $R_{ch}$ values on the x-axis from 2.1 to 2.7.

**Graph 2:**
- $^{40}\text{Ca}$
- Similar to Graph 1, but with $\alpha_D$ values from 0.4 to 2.4,
- $R_{ch}$ values from 2.2 to 3.6.

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Tuesday, 15 September, 15
Electric Dipole Polarizability

with 3N forces ★ NNLO_{sat}

Much better agreement with experimental data
Results for $^{48}\text{Ca}$

Hagen et al., (2015)

- $\text{NNLO}_{\text{sat}}$
- Soft NN(N$^3\text{LO}$)+3N(N$^2\text{LO}$) Hebeler et al.
- Density Functional Theory
Results for $^{48}$Ca

Hagen et al., (2015)

Exploiting correlations among observables and the very precise measurement of $R_p$, we predict:

\[ 0.12 \leq R_{\text{skin}} \leq 0.15 \text{ fm} \]

- Will be measured at JLab by CREX with parity-violation electron scattering

\[ 2.19 \leq \alpha_D \leq 2.60 \text{ fm}^3 \]

- Being measured at RCNP (Osaka) with $(p,p')$

\[ \text{NNLO}_{\text{sat}} \]
\[ \text{Soft NN(N}^3\text{LO)+3N(N}^2\text{LO) Hebeler et al.} \]
\[ \text{Density Functional Theory} \]
Conclusions and Outlook

- Electromagnetic observables are key to test our understanding of nuclear forces
- Extending first principles calculations to medium mass nuclei is possible and very exciting: more applications/impact on experiments in the future
- Monopole strengths, M1 and GT teller transitions

Thanks to my collaborators:

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M. Hjorth-Jensen, G. R. Jansen, W. Leidemann, M. Miorelli, W. Nazarewicz, G. Orlandini,
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T. Papenbrock, J. Simonis, A. Schwenk, K. Went

Thank you!
Backup
The inversion is performed numerically with a regularization procedure

**Ansatz**

\[
R(\omega) = \sum_{i}^{I_{\text{max}}} c_i \chi_i(\omega, \alpha) \\
L(\sigma, \Gamma) = \sum_{i}^{I_{\text{max}}} c_i \mathcal{L}[\chi_i(\omega, \alpha)]
\]

Least square fit of the coefficients \(c_i\) to reconstruct the response function

**Message:** using bound-states techniques to calculate the LIT is correct and inversions are stable
New theoretical method aimed at extending \textit{ab-initio} calculations towards medium-mass

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

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

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

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

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

$L(\sigma, \Gamma) = \langle \tilde{\Psi} |\tilde{\Psi}\rangle =$

\[-\frac{1}{2\pi} \Im \left\{ \langle \tilde{\Psi}_L |\Theta^\dagger \left[ |\tilde{\Psi}_R(z^*)\rangle - |\tilde{\Psi}_R(z)\rangle \right] \right\}\]

with $|\tilde{\Psi}_R(z^*)\rangle = \hat{R}(z^*) |\Phi_0\rangle$

Equation of Motion with source No approximations done so far!

Formulation based on the solution of an

Present implementation in the CCSD scheme

\begin{equation}
T = T_1 + T_2
\end{equation}

\begin{equation}
\hat{R} = \hat{R}_0 + \hat{R}_1 + \hat{R}_2
\end{equation}
Extension to $^{16}$O with NN forces derived from chiral EFT (N$^3$LO)

Convergence in the model space expansion

Good convergence

Small HO dependence: use it as error bar
Giant Dipole Resonances

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

$\sigma(\omega)/(4\pi^2 \alpha \omega)$ [mb/MeV]

$^{16}\text{O}$

- △ Ahrens et al.
- ● Ishkanov et al.
- Blue line: CCSD

Lyutorovich et al., PRL 109 092502 (2012)
with Skyrme functionals
Validation for $^4$He: comparison with exact hyperspherical harmonics

NN forces derived from chiral EFT (N$^3$LO)

Miorelli et al., in preparation

The comparison with exact theory is very good
Small difference due to missing triples and quadruples
Electric Dipole Polarizability

Medium-mass nuclei with NN(N³LO)  M. Miorelli et al., in preparation (2015)

\[ D = 0.46 \text{ fm}^3 \]
\[ D^{\text{exp}} = 0.585(9) \text{ fm}^3 \]

\[ R_{\text{ch}} = 2.3 \text{ fm} \]
\[ R^{\text{exp}}_{\text{ch}} = 2.6991(52) \text{ fm} \]

\[ \alpha_D = 0.46 \text{ fm}^3 \]
\[ \alpha^{\text{exp}}_D = 0.585(9) \text{ fm}^3 \]

\[ R_{\text{ch}} = 3.05 \text{ fm} \]
\[ R^{\text{exp}}_{\text{ch}} = 3.4776(19) \text{ fm} \]

The present Hamiltonian underestimates both radii and electric dipole polarizabilities
Giant Dipole Resonance in $A=6$

with Hyperspherical Harmonics

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

$$E1 = \sum_i^Z (z_i - Z_{cm})$$

$^6\text{Li}$ stable

$^6\text{He}$ unstable $T_{1/2} = 806$ ms

NSCL, Wang et al.
GSI, Aumann et al.

Soft Dipole Mode