

Electromagnetic observables from coupled-cluster theory

Sonia Bacca

Johannes Gutenberg Universität Mainz and TRIUMF

March 1st, 2018

Strength functions

Example: dipole strength function



Strength functions

Example: dipole strength function



Continuum problem

$$R(\omega) = \sum_{f} \left| \left\langle \psi_{f} \left| \Theta \right| \psi_{0} \right\rangle \right|^{2} \delta(E_{f} - E_{0} - \omega)$$

Depending on $\,E_{\rm f}$, many channels may be involved



How do we address it?

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

$$\Gamma \qquad L(\sigma,\Gamma) = \frac{\Gamma}{\pi} \int d\omega \frac{R(\omega)}{(\omega-\sigma)^2 + \Gamma^2}$$

$$(H - E_0 - \sigma + i\Gamma) \mid \tilde{\psi} \rangle = \Theta \mid \psi_0 \rangle$$

How do we address it?

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

How do we address it?

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

Photonuclear reactions

S.B. et al., Phys. Rev. Lett. 111, 122502 (2013)

$$(\bar{H} - E_0 - \sigma + i\Gamma) |\tilde{\Psi}_R\rangle = \bar{\Theta} |\Phi_0\rangle$$

$$\bar{H} = e^{-T} H e^{T}$$
$$\bar{\Theta} = e^{-T} \Theta e^{T}$$
$$|\tilde{\Psi}_R\rangle = \hat{R} |\Phi_0\rangle$$

Implementation at the singles and doubles level

S.B. et al., Phys. Rev. C 90, 064619 (2014)



Sum rules

$$m_n = \int_0^\infty d\omega \,\,\omega^n R(\omega) = \langle \Psi_0 | \hat{\Theta}^\dagger (\hat{H} - E_0)^n \hat{\Theta} | \Psi_0 \rangle$$

Sum rules

$$m_n = \int_0^\infty d\omega \,\,\omega^n R(\omega) = \langle \Psi_0 | \hat{\Theta}^\dagger (\hat{H} - E_0)^n \hat{\Theta} | \Psi_0 \rangle$$

Bremsstrahlung sum rule $m_0 = \langle \Phi_0 | (1 + \Lambda) \overline{\Theta}_N^{\dagger} \cdot \overline{\Theta}_N | \Phi_0 \rangle$

Polarizability sum rule
$$\alpha_D = 2\alpha m_{-1} = 2\alpha \lim_{\Gamma \to 0} \langle \Phi_0 | (1+\Lambda)\overline{\Theta}_N^{\dagger} \frac{1}{\overline{H} - E_0 - i\Gamma} \overline{\Theta}_N | \Phi_0 \rangle$$

Sum rules

$$m_n = \int_0^\infty d\omega \,\,\omega^n R(\omega) = \langle \Psi_0 | \hat{\Theta}^\dagger (\hat{H} - E_0)^n \hat{\Theta} | \Psi_0 \rangle$$

Bremsstrahlung sum rule $m_0 = \langle \Phi_0 | (1 + \Lambda) \overline{\Theta}_N^{\dagger} \cdot \overline{\Theta}_N | \Phi_0 \rangle$

Polarizability sum rule
$$\alpha_D = 2\alpha m_{-1} = 2\alpha \lim_{\Gamma \to 0} \langle \Phi_0 | (1+\Lambda)\overline{\Theta}_N^{\dagger} \frac{1}{\overline{H} - E_0 - i\Gamma} \overline{\Theta}_N | \Phi_0 \rangle$$

Coupled cluster expansions

$$T,\Lambda$$
 ground-state \Longrightarrow affecting $\bar{\Theta}_N$

R,L excited-states (EoM)

Running sum rule



Full triples are prohibitive

We will use linearized triples for ground state and EoM $T_3 = f(T_1, T_2)$

Full triples are prohibitive

We will use linearized triples for ground state and EoM $T_3 = f(T_1, T_2)$

Similarity transformed operator

M. Miorelli, PhD Thesis (2017) M. Miorelli *et al.,* in preparation (2018)

$$\bar{\Theta}_N = \left[\Theta_N e^{T_1 + T_2 + T_3}\right]_C = \bar{\Theta}_N^D + \left[\Theta_N \left(\frac{T_2^2}{2} + T_3 + T_1 T_3\right)\right]_C$$
$$\simeq \bar{\Theta}_N^D + \left[\Theta_N \left(\frac{T_2^2}{2}\right)\right]_C$$
$$\simeq \bar{\Theta}_N^D$$

Full triples are prohibitive

We will use linearized triples for ground state and EoM $T_3 = f(T_1, T_2)$

Similarity transformed operator

M. Miorelli, PhD Thesis (2017) M. Miorelli *et al.,* in preparation (2018)

	⁴ He	¹⁶ O
$\lceil /T^2 \rangle$)]	$m_0[\mathrm{fm}]$	
$\bar{\Theta}_N = \left[\Theta_N e^{T_1 + T_2 + T_3}\right]_C = \bar{\Theta}_N^D + \left[\Theta_N \left(\frac{T_2}{2} + T_3 + T_1 T_3\right)\right]_C$	0.951	4.87
$\simeq \bar{\Theta}_N^D + \left[\Theta_N\left(\frac{T_2^2}{2}\right)\right]$	0.950	4.92
$\simeq \bar{\Theta}_N^D$	0.949	4.90

Full triples are prohibitive

We will use linearized triples for ground state and EoM $T_3 = f(T_1, T_2)$

Similarity transformed operator M. Miorelli, PhD Thesis (2017)

M. Miorelli, PhD Thesis (2017) M. Miorelli *et al.,* in preparation (2018)

	⁴ He	¹⁶ O
$\lceil /T^2 \rangle$)]	m_0 [fm]	
$\bar{\Theta}_N = \left[\Theta_N e^{T_1 + T_2 + T_3}\right]_C = \bar{\Theta}_N^D + \left[\Theta_N \left(\frac{T_2}{2} + T_3 + T_1 T_3\right)\right]_C$	0.951	4.87
$\simeq \bar{\Theta}_N^D + \left[\Theta_N\left(\frac{T_2^2}{2}\right)\right]$	0.950	4.92
$\simeq \bar{\Theta}_N^D$	0.949	4.90

By using only $\bar{\Theta}_N^D$ you are missing 0.2 - 0.6% of the strength only

Much simpler and the only feasible calculation in heavy nuclei

Benchmark

M. Miorelli et al., in preparation (2018)

Hyperspherical harmonics (HH) contain all correlations (up to quadruples)



Comparison with experiment and theory

M. Miorelli et al., in preparation (2018)

Experimental data from photoabsorption cross sections



Comparison with experiment and theory

M. Miorelli et al., in preparation (2018)

Experimental data from photoabsorption cross sections



Comparison with experiment and theory

M. Miorelli et al., in preparation (2018)

Experimental data from photoabsorption cross sections



Barbieri et al., arXiv:1711.04698 SCGF approach obtains 0.50 fm³ comparable to D/S giving 0.502 fm³

Chiral convergence

J. Simonis et al. (2018)



EMN: Entem, Machleidt and Nosyk, PRC 96, 024004(2017)

This will help shed light on systematic uncertainties in muonic ⁴He (see talks by Hernandez and Nevo Dinur)

Coulomb sum rule

k'^μ

Total strength of inelastic longitudinal response function



Coulomb sum rule

S. Bacca et al., in preparation (2018)





Outlook

• Triples-correlations:

Corrections beyond D in the similarity transformed operator are negligible The T-1/D approximation agrees with exact results and coincidentally with D/S

- Work in progress in analyzing the chiral convergence and the Coulomb sum rule
- In the future we plan to address electron-nucleus and neutrino-nucleus scattering B. Acharya

Outlook

• Triples-correlations:

Corrections beyond D in the similarity transformed operator are negligible The T-1/D approximation agrees with exact results and coincidentally with D/S

- Work in progress in analyzing the chiral convergence and the Coulomb sum rule
- In the future we plan to address electron-nucleus and neutrino-nucleus scattering B. Acharya

Thanks to all my collaborators

G. Hagen, M. Miorelli, J. Simonis, T. Papenbrock, et al.

Outlook

• Triples-correlations:

Corrections beyond D in the similarity transformed operator are negligible The T-1/D approximation agrees with exact results and coincidentally with D/S

- Work in progress in analyzing the chiral convergence and the Coulomb sum rule
- In the future we plan to address electron-nucleus and neutrino-nucleus scattering B. Acharya

Thanks to all my collaborators

G. Hagen, M. Miorelli, J. Simonis, T. Papenbrock, et al.

Thanks for your attention!

Backup

Work from J. Simonis (2018)

NB: Stange behaviour observed at LO with cutoff 550 MeV

