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Canada's national laboratory for particle and nuclear physics
Laboratoire national canadien pour la recherche en physique nucléaire
et en physique des particules

Towards ab-initio calculations of electromagnetic reactions in medium-mass nuclei

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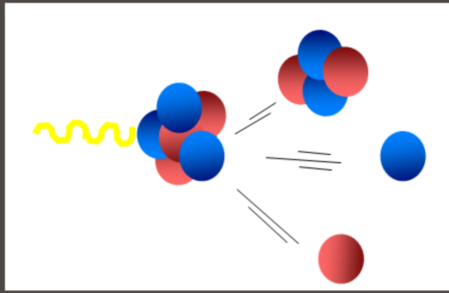
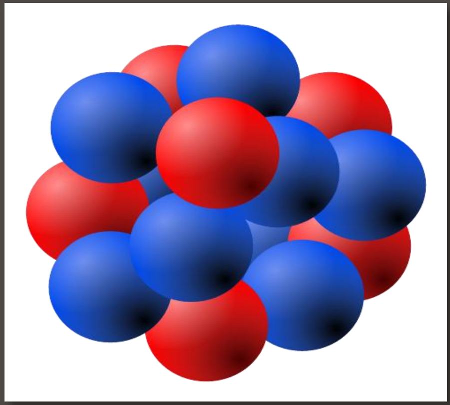
February 20th, 2013

UBC a place of mind THE UNIVERSITY OF BRITISH COLUMBIA



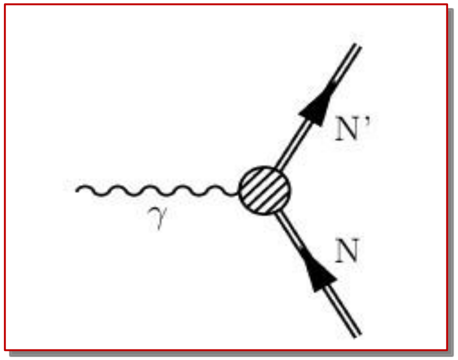
Nuclear Reactions



$^{16}O, ^{40}Ca, ^{48}Ca$

Photo-absorption Reactions

Photo-absorption reactions



We focus on the low-energy continuum region of the spectrum, we want to study:

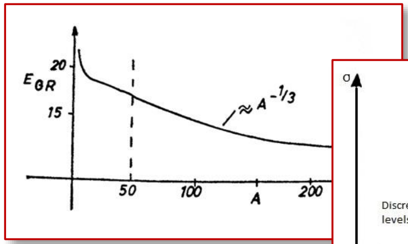
- **Giant Dipole Resonance (GDR)**

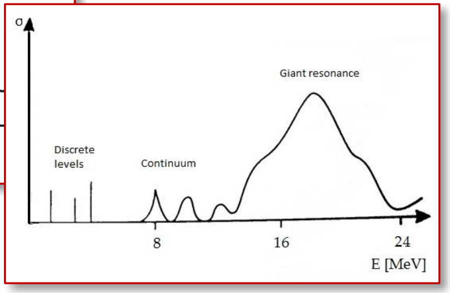
- **Electric Dipole Polarizability (EDP)**

GDR and EDP

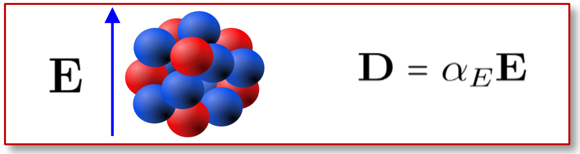
The Giant Dipole Resonance (GDR)

- Common feature of the photo-absorption cross-section of all nuclei
- The position of the peak depends on the mass number





The Electric Dipole Polarizability (EDP)



- Interesting for the study of neutron-rich matter
- Ongoing experiment on ^{48}Ca polarizability at RCNP[*] and neutron-skin radius experiments at JLAB[**]

[*] Tamii A. et al., Phys. Rev. Lett. 107, 062502 (2011)
[**] Calcium Radius Experiment (CREX) Workshop at Jefferson Lab, March 17-19, 2013, Mammei J. et al., CREX, http://hallaweb.jlab.org/parity/prex/c-rex2013_v7.pdf

Theoretical Approach

Current situation on the theoretical description:

- **Non-ab-initio**: via macroscopic models or mean field based methods
- **Ab-initio**: described via exact computations for light nuclei using the LIT+EIHH method (up to A =7)

No ab-initio description of the GDR for A>7
→ need of a new approach for larger nuclei

What ingredients and tools do we need?

- **Nuclear interactions** → ChPT
- **Continuum problem** → LIT
- **Many-body technique** → CC

LIT Method

The response function $R(\omega)$ is the key quantity

$$\sigma_\gamma(\omega) = 4\pi^2 \alpha \omega R(\omega)$$

$$\alpha_E = 2\alpha \int d\omega \frac{R(\omega)}{\omega}$$

$$R(\omega) = \sum\!\!\!\!\!\!\!\int_f |\langle f|\hat{\theta}|i\rangle|^2 \delta(E_f - E_i - \omega)$$

- Final states problem is tackled with the Lorentz Integral Transform (LIT) method

$$L(\omega_0, \Gamma) = \frac{\Gamma}{\pi} \int d\omega \frac{R(\omega)}{(\omega_0 - \omega)^2 + \Gamma^2}$$

where $(H - E_i + \sigma)|\tilde{\psi}\rangle = \theta|i\rangle$ and $\sigma = -\omega_0 - i\Gamma$

$$L(\sigma) = \frac{\Gamma}{\pi} \langle i|\theta^+ (H - E_i + \sigma^*)^{-1} (H - E_i + \sigma)^{-1} \theta|i\rangle = \langle\tilde{\psi}|\tilde{\psi}\rangle < \infty$$

- The exact final state interaction is included in the continuum rigorously!

$$L(\sigma) \xrightarrow{Inversion} R(\omega)$$

CC Theory

- Continuum problem → Bound state problem

$$L(\sigma) = \frac{\Gamma}{\pi}\langle i|\theta^{+}(H - E_i + \sigma^{*})^{-1}(H - E_i + \sigma)^{-1}\theta|i\rangle$$

- Computation of the ground state → **Coupled Cluster (CC) theory**

$$|i\rangle = e^{T}|0\rangle$$

$$\mathrm{T} = \sum_{i=1}^{A} T_i$$

$$T_n = \frac{1}{(n!)^2}\sum_{\substack{a_1,a_2,\dots,a_n\\ i_1,i_2,\dots,i_n}} t_{i_1 i_2 \dots i_n}^{a_1 a_2 \dots, a_n}\{a_1^{+} i_1 a_2^{+} i_2 \dots a_n^{+} i_n\}$$

Ground state energy $E_i = \langle 0|\bar{H}|0\rangle$

$\bar{H} = e^{-T} H_N e^{T}$ Symilarity transformed Hamiltonian

- The T amplitudes are found solving a set of non-linear coupled equations

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LIT Method + CC Theory

- **We use the exponential ansatz of CC theory with the response function from LIT method:**

LIT

$$L(\sigma) = -\frac{i}{2\Gamma}\left[\langle i|\theta^+|\tilde{\psi}(\sigma)\rangle - \langle i|\theta^+|\tilde{\psi}(\sigma^*)\rangle\right]$$

$$(H - E_0 + \sigma)|\tilde{\psi}(\sigma)\rangle = \theta|i\rangle$$

$$H \rightarrow \bar{H} = e^{-\hat{T}} H_N e^{\hat{T}}$$

$$\theta \rightarrow \bar{\theta} = e^{-\hat{T}} \theta_N e^{\hat{T}}$$

LIT + CC

$$L(\sigma) = -\frac{i}{2\Gamma}\left[\langle 0_L|\bar{\theta}^+|\tilde{\psi}_R(\sigma)\rangle - \langle 0_L|\bar{\theta}^+|\tilde{\psi}_R(\sigma^*)\rangle\right]$$

$$(\bar{H} - \Delta E_0 + \sigma)|\tilde{\psi}_R(\sigma)\rangle = \bar{\theta}|0_R\rangle$$

LIT Method + CC Theory

Coupled Cluster Equation of Motion (CC-EOM) method

$$L(\sigma) = -\frac{i}{2\Gamma}\left[\langle 0_L|\bar{\theta}^{+}|\tilde{\psi}_R(\sigma)\rangle - \langle 0_L|\,\bar{\theta}^{+}|\,\tilde{\psi}_R(\sigma^{*})\rangle\right]$$

+

$$\left|\tilde{\psi}_R(\sigma)\right\rangle = R(\sigma)|0_R\rangle$$

$$R(\sigma) = r_0(\sigma) + \sum_{a,i} r_i^{a}(\sigma)\{c_a^{+}c_i\} + \frac{1}{4}\sum_{ab,ij} r_{ij}^{ab}(\sigma)\left\{c_a^{+}c_i c_b^{+}c_j\right\} + \cdots$$

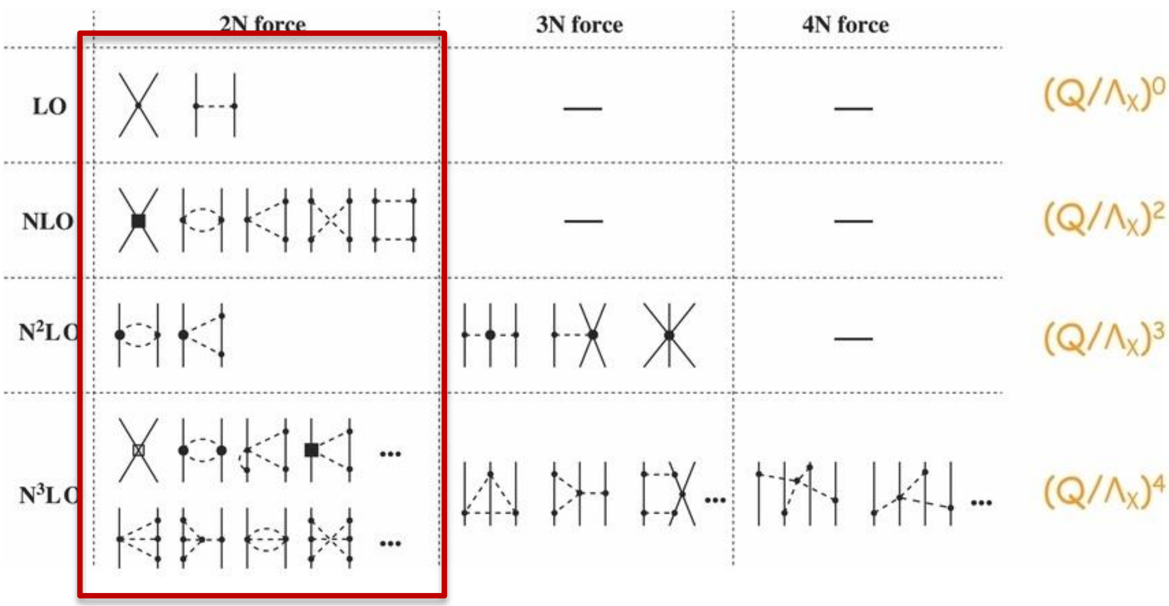
↓

$$L(\sigma) = -\frac{i}{2\Gamma}\langle 0_L\left|\bar{\theta}^{+}[R(\sigma) - R(\sigma^{*})]\right|0_R\rangle$$

$R(\sigma)$ ← $(\bar{H}R(\sigma) - R(\sigma)\bar{H})|0_R\rangle = -\sigma R(\sigma)|0_R\rangle + \bar{\theta}|0_R\rangle$

Application of LIT+CC Method

R. Machleidt and D. Entem, Phys. Rep. 503, 1 (2011)



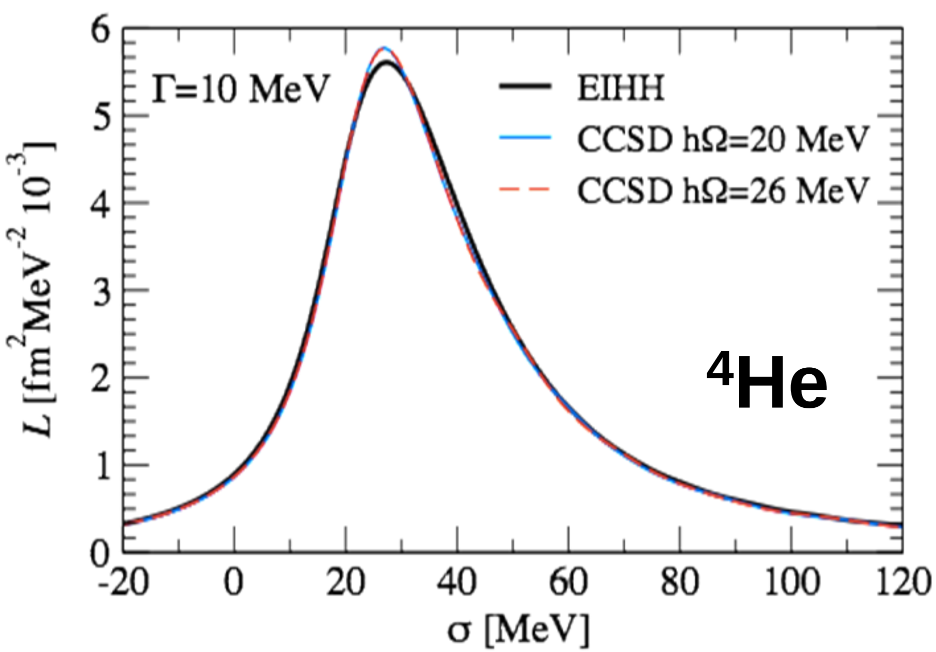
- **2NF up to N3LO**
- **CCSD approximation**

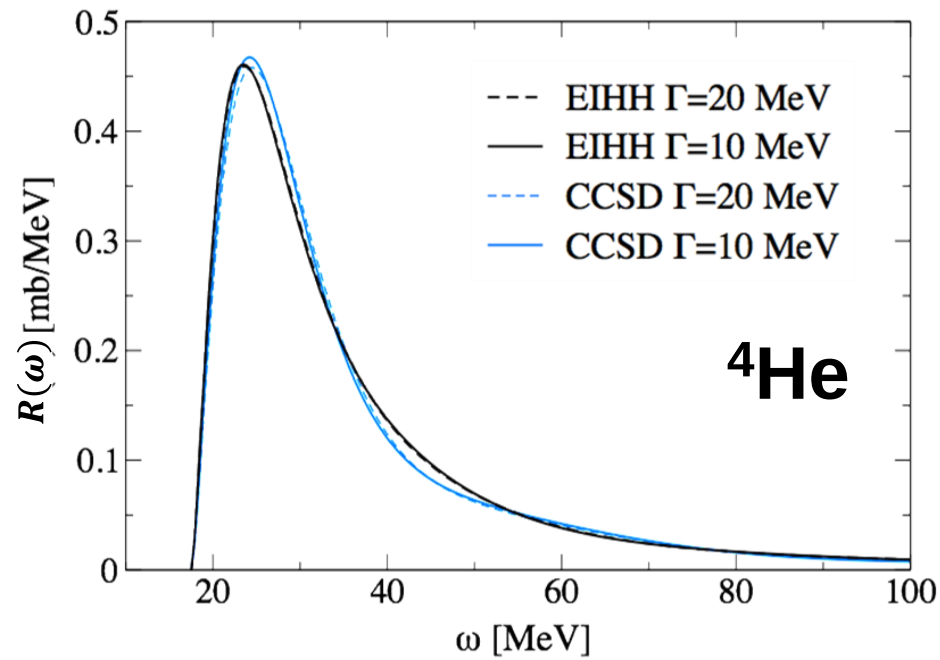
$$T = T_1 + T_2 \qquad R(\sigma) = R_0(\sigma) + R_1(\sigma) + R_2(\sigma)$$

^{4}He and ^{16}O

Validation of LIT+CC method with previous results obtained using LIT+EIHH method

Bacca, S., N. Barnea, G. Hagen, G. Orlandini, and T. Papenbrock (2013), Phys. Rev. Lett. 111, 122502.

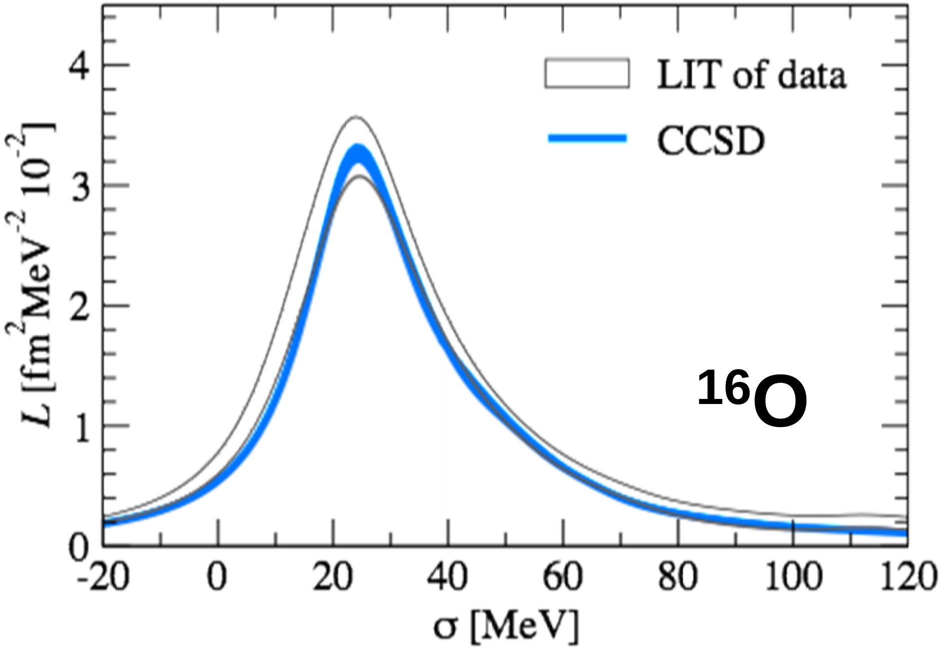




- Overall good agreement
- Discrepancies due truncation to CCSD

^{4}He and ^{16}O

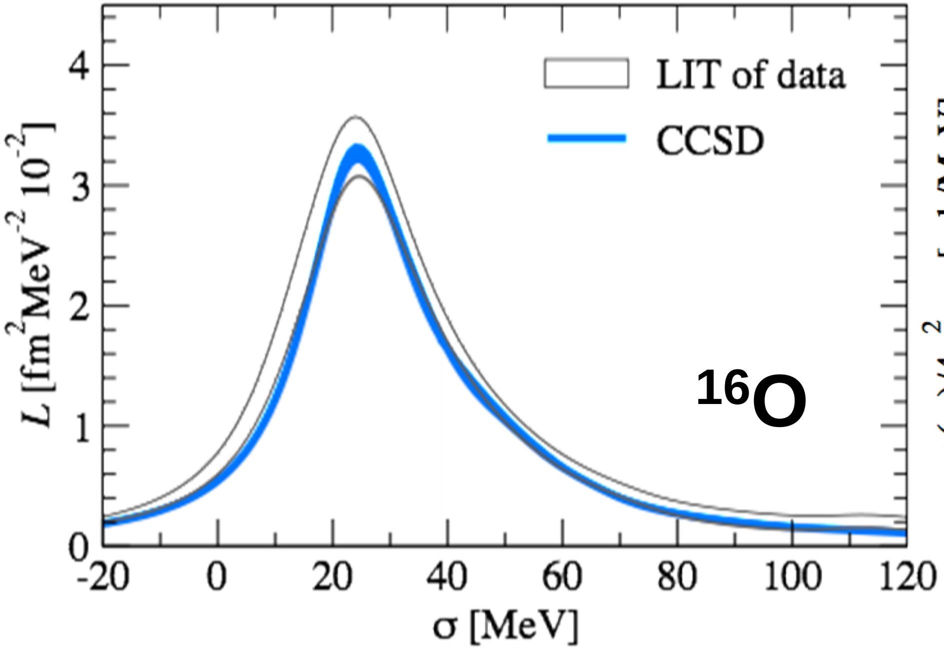
Bacca, S., N. Barnea, G. Hagen, G. Orlandini, and T. Papenbrock (2013), Phys. Rev. Lett. 111, 122502.

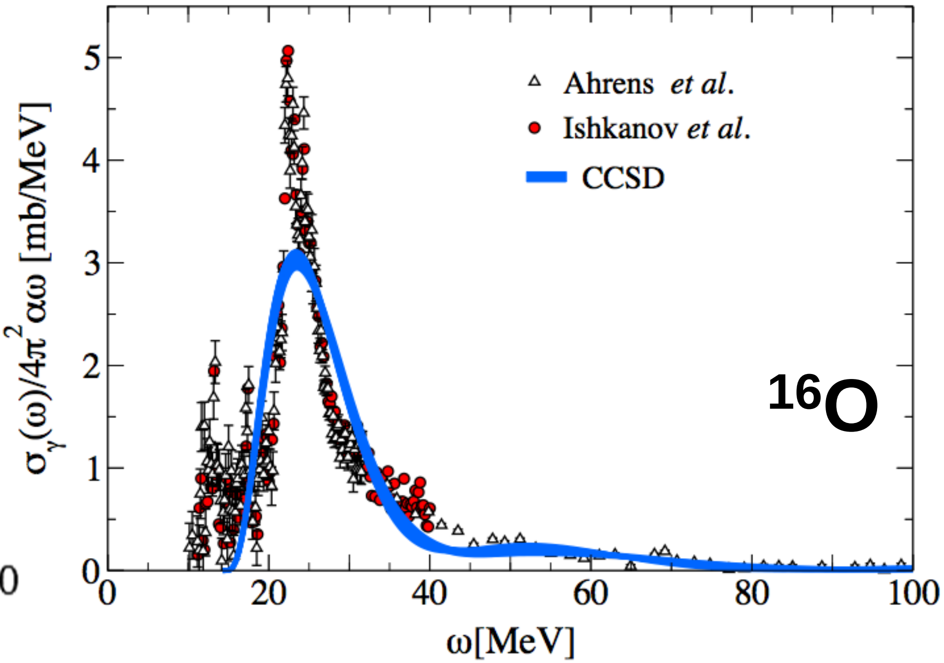


- Total strength and position of the GDR reproduced quite well

^{4}He and ^{16}O

Bacca, S., N. Barnea, G. Hagen, G. Orlandini, and T. Papenbrock (2013), Phys. Rev. Lett. 111, 122502.





- Total strength and position of the GDR reproduced quite well

- The GDR of ^{16}O is described from first principles for the first time!

The Electric Dipole Polarizability

In preparation...

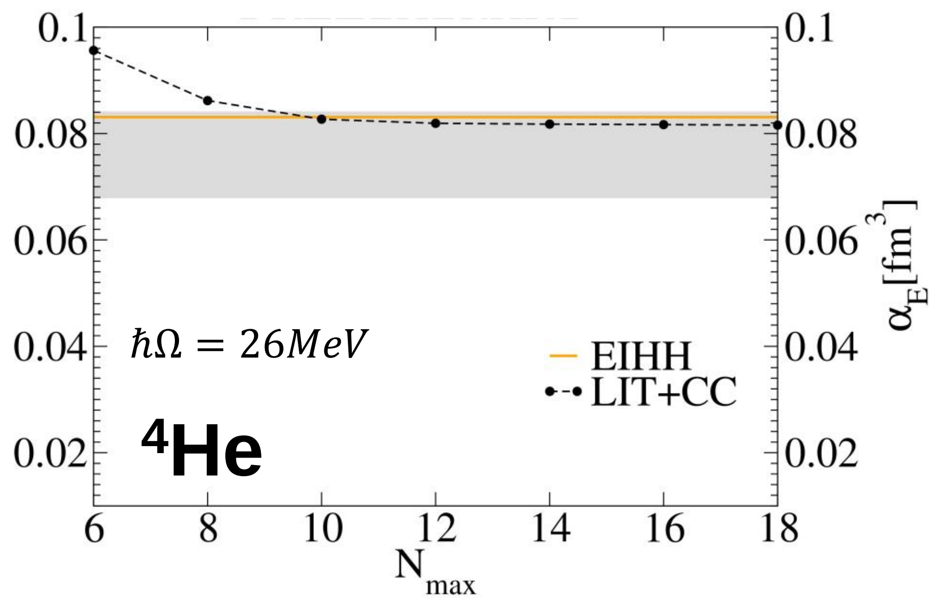
M. M., G. Orlandini, S. Bacca, N. Barnea, G. Hagen and T. Papenbrock

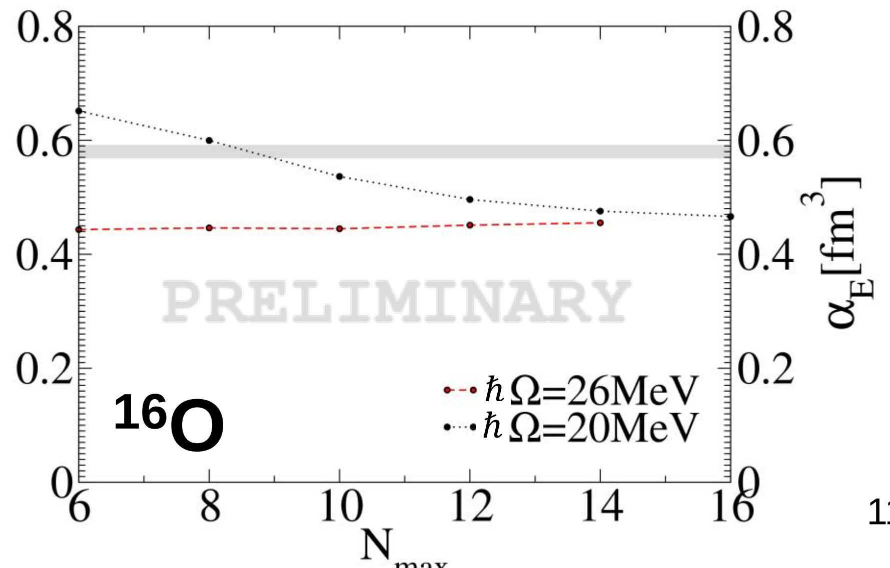
$$\alpha_E = 2\alpha \int \frac{R(\omega)d\omega}{\omega}$$

otherwise

α_E can be obtained when computing $L(\sigma)$ (Lanczos method)

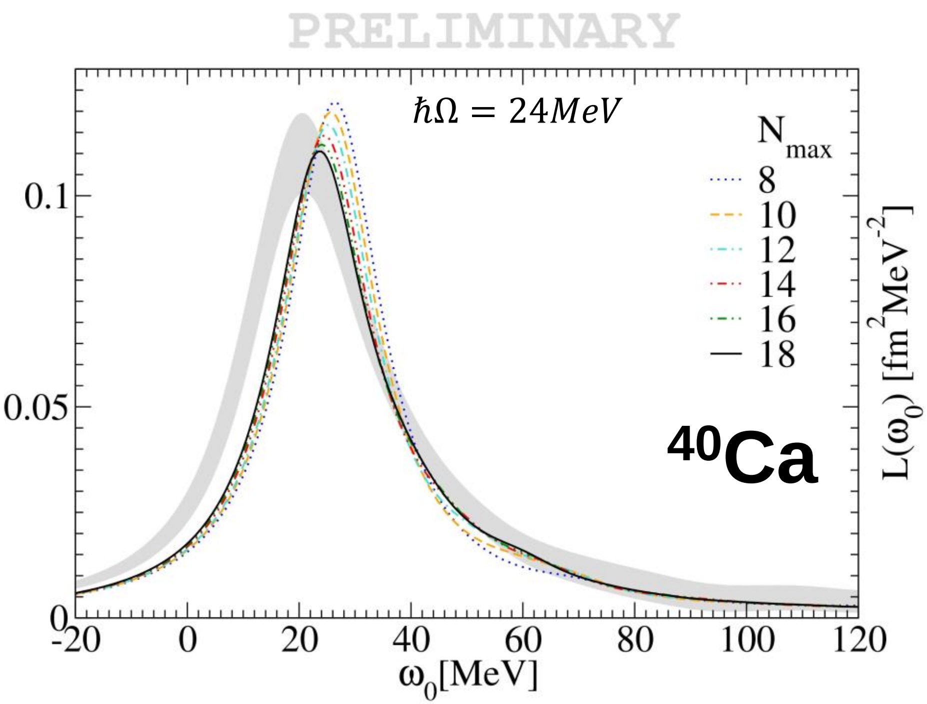
No inversion is required

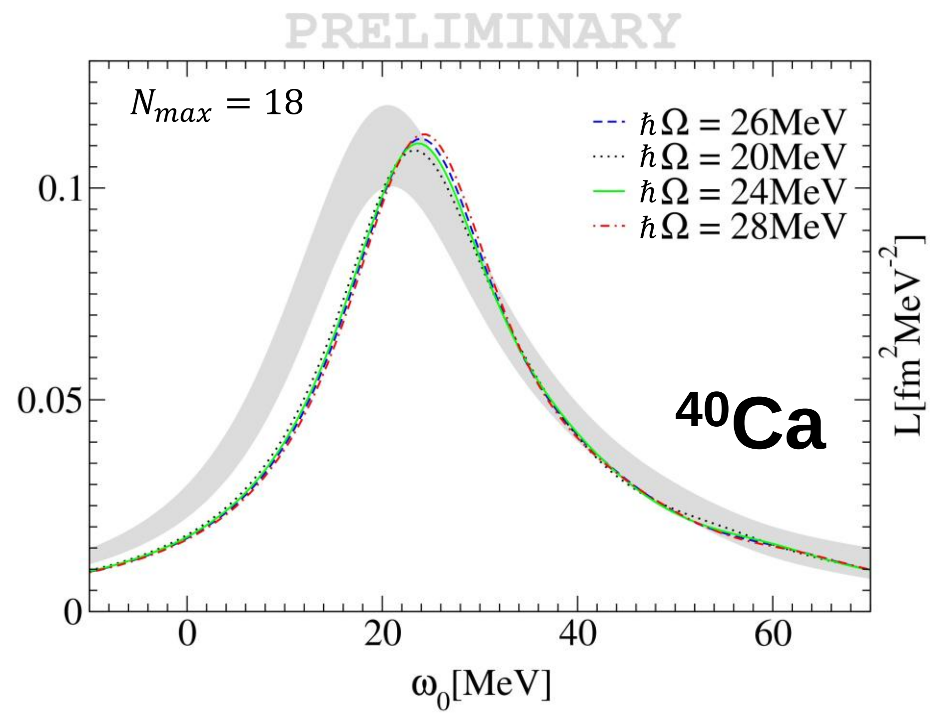




Work in progress: ^{40}Ca and ^{48}Ca

Orlandini, G., S. Bacca, N. Barnea, G. Hagen, M. M., and T. Papenbrock (2013),ArXiv e-prints arXiv:1311.2141 [nucl-th]





- The convergence of the LIT is approached
- The peak position of the computed LIT is about 4MeV shifted on the right with respect to the LIT of experimental data

Work in progress: ^{40}Ca and ^{48}Ca

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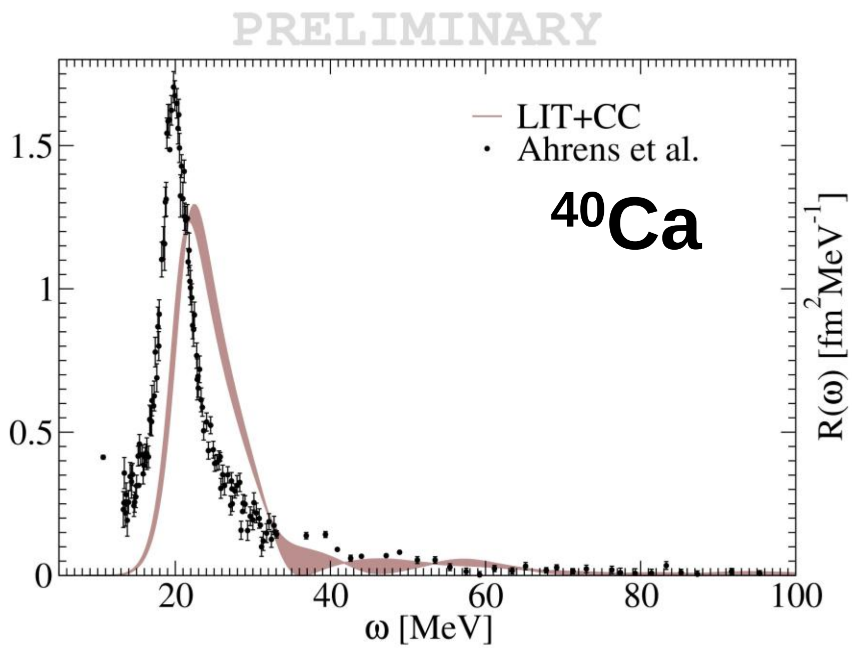
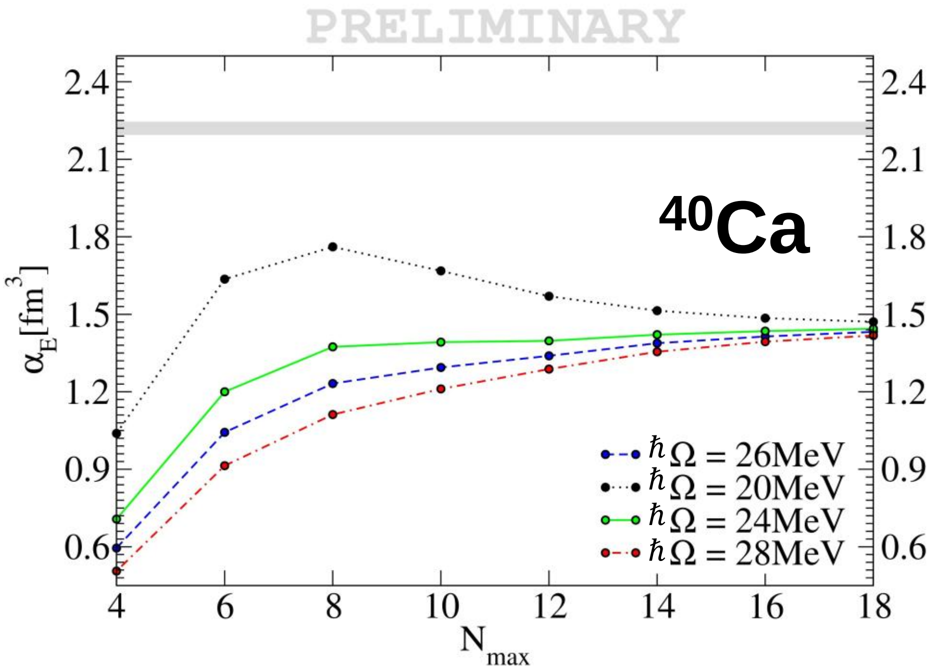


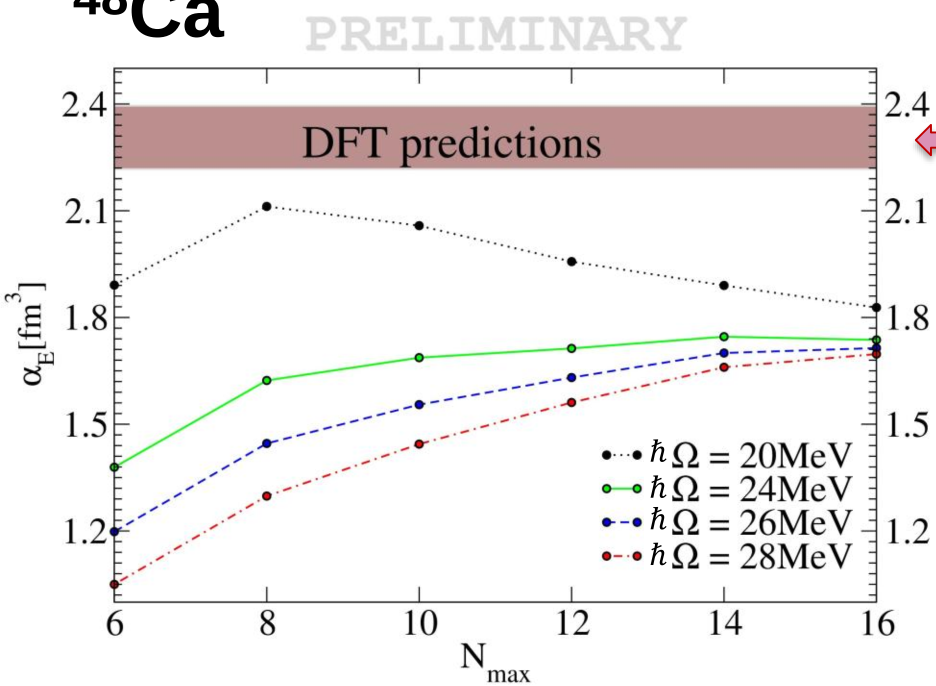


- As expected from the computed LIT, also the response function peak is shifted to the right
- The electric dipole polarizability is underestimated with respect to the experimental value

Work in progress: ^{40}Ca and ^{48}Ca

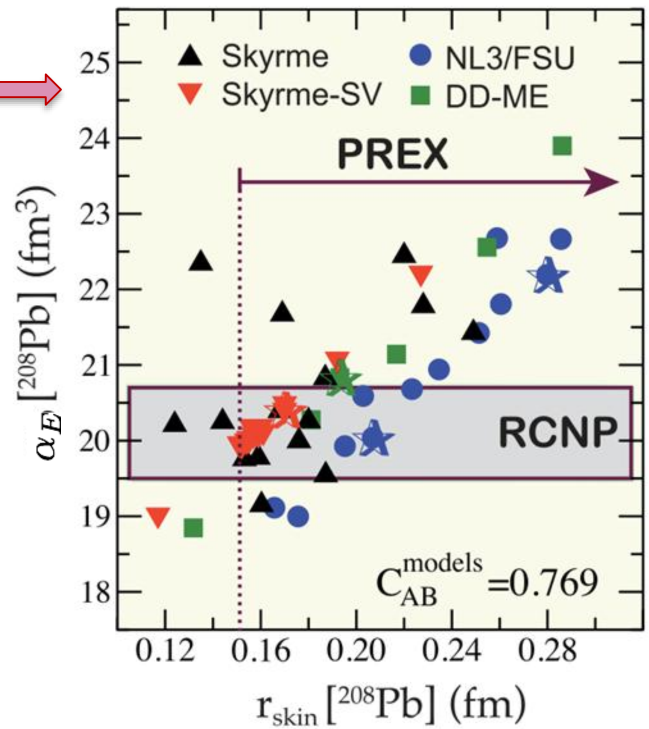
^{48}Ca

Towards an ab-initio theory for ^{48}Ca



Phys. Rev. C 85, 041302 (2012)

Energy Density Functional Theory



- α_E is very correlated to r_{skin}
- Future insight from RCNP and JLAB(CREX) experiments

Summary and Outlook

- We can extend the LIT method to heavier nuclei using the CC theory
- The GDR and EDP of ^{16}O, ^{40}Ca and the EDP of ^{48}Ca have been computed with a first principles based method for the first time

Future perspectives:

- Improve the method by adding:
  - 3NF in the Hamiltonian
  - triple excitations in the cluster operator of CC theory
- Investigate the relation between the electric dipole polarizability and the neutron skin radius
- We aim to provide deep insight in future and ongoing experiments (RCNP and JLAB(CREX))

Thank you!
Merci

Lanczos method

$$L(\sigma) = -\frac{i}{2\Gamma}\langle 0_L|\hat{\bar{\theta}}^\dagger(\hat{R}(\sigma) - \hat{R}(\sigma^*))|0_R\rangle$$

$$L(\sigma) = -\frac{i}{2\Gamma}((\mathbf{S}^L)^\dagger \cdot \mathbf{S}^R)\mathbf{w}_0^T\left\{(\mathbb{M} + \mathbb{I}\sigma)^{-1} - (\mathbb{M} + \mathbb{I}\sigma^*)^{-1}\right\}\mathbf{v}_0$$

$$\mathbf{v}_0 = \frac{\mathbf{S}^R}{\sqrt{(\mathbf{S}^L)^\dagger \cdot \mathbf{S}^R}}$$

$$\mathbf{w}_0^T = \frac{(\mathbf{S}^L)^\dagger}{\sqrt{(\mathbf{S}^L)^\dagger \cdot \mathbf{S}^R}}$$

$$\mathbb{M} = \begin{pmatrix} 0 & \langle 0_R|[\hat{\bar{H}}, N[a_d^\dagger a_k]]|0_R\rangle & \langle 0_R|[\hat{\bar{H}}, N[c_d^\dagger c_k c_e^\dagger c_l]]|0_R\rangle & \cdots \\ 0 & \langle \phi_i^a||[\hat{\bar{H}}, N[c_d^\dagger c_k]]|0_R\rangle & \langle \phi_i^a|[\hat{\bar{H}}, N[c_d^\dagger c_k c_e^\dagger c_l]]|0_R\rangle & \cdots \\ 0 & \langle \phi_{ij}^{ab}|[\hat{\bar{H}}, N[c_d^\dagger c_k]]|0_R\rangle & \langle \phi_{ij}^{ab}|[\hat{\bar{H}}, N[c_d^\dagger c_k c_e^\dagger c_l]]|0_R\rangle & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix}$$

$$\hat{R}(\sigma^*) = r_0(\sigma^*) + \sum_{i,a} r_i^a(\sigma^*)N[c_a^\dagger c_i] + \sum_{ij,ab} r_{ij}^{ab}(\sigma^*)N[c_a^\dagger c_i c_b^\dagger c_j] + \ldots$$

$$(\mathbf{S}^L)^\dagger = \left(\langle 0_L|\hat{\bar{\theta}}^\dagger|0_R\rangle, \langle 0_L|\hat{\bar{\theta}}^\dagger|\phi_i^a\rangle, \langle 0_L|\hat{\bar{\theta}}^\dagger|\phi_{ij}^{ab}\rangle, \ldots\right)$$

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Lanczos method

- Use Lanczos do diagonalize (avoid full direct diagonalization)

$$L(\sigma) = -\frac{i}{2\Gamma}((\mathbf{S}^L)^\dagger \cdot \mathbf{S}^R)\left(X_0(\sigma) - X_0(\sigma^*)\right)$$

$$X_0(\sigma) = \cfrac{1}{(a_0+\sigma) - \cfrac{b_1^2}{(a_1+\sigma) - \cfrac{b_2^2}{(a_2+\sigma) - \cfrac{b_3^2}{\cdots}}}}$$

- The Electric Dipole Polarizability is obtained in a similar way directly from the Lanczos coefficients of the Lanczos tridiagonal matrix

$$\begin{aligned}\alpha_E &= 2\alpha \lim_{\sigma_R \to 0} \int \frac{R(\omega)d\omega}{\omega + \sigma_R} \\ &= 2\alpha \lim_{\sigma_R \to 0} \sum\!\!\!\!\!\!\int_f \frac{\langle 0_L| e^{-\hat{T}} \hat{\theta}_N^\dagger |f\rangle \langle f| \hat{\theta}_N e^{\hat{T}} |0_R\rangle}{\Delta E_f - \Delta E_0 + \sigma_R} \\ &= 2\alpha \lim_{\sigma_R \to 0} \langle 0_L | \hat{\bar{\theta}}^\dagger [\hat{\bar{H}} - \Delta E_0 + \sigma_R]^{-1} \hat{\bar{\theta}} | 0_R \rangle .\end{aligned}$$

$$\alpha_E = 2\alpha((\mathbf{S}^L)^\dagger \cdot \mathbf{S}^R) \lim_{\sigma_R \to 0} X_0(\sigma_R)$$