

Canada's National Laboratory for Particle and Nuclear Physics Laboratoire national canadien pour la recherche en physique nucléaire et en physique des particules

# First Principle Calculation of Nuclear Response Functions

#### Sonia Bacca

#### **TRIUMF Theory Group**

INT program on "Computational and Theoretical advances for Exotic isotopes in the Medium Mass Region" April 19, 2013

Owned and operated as a joint venture by a consortium of Canadian universities via a contribution through the National Research Council Canada Propriété d'un consortium d'universités canadiennes, géré en co-entreprise à partir d'une contribution administrée par le Conseil national de recherches Canada







## **Electro-weak reactions**

The coupling constant << 1</li>
 *main of the coupling constant << 1*

"With the electro-weak 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"  $\sigma \propto \left| \langle \psi_f | \hat{J}^\mu | \psi_0 \rangle \right|^2$ [De Forest-Walecka, Ann. Phys. 1966]

$$\sigma \propto R(q,\omega) \quad \text{with} \quad R(q,\omega) = \sum_{f} \left| \left\langle \psi_{f} | \hat{J}^{\mu}(q) | \psi_{0} \right\rangle \right|^{2} \delta(\underline{E_{f}} - E_{0} - \omega)$$

**Nuclear Response Function** 



## From "First Principles"

- 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

 $H|\psi\rangle = E|\psi\rangle$ 

 $H = T + V_{NN}(\Lambda) + V_{3N}(\Lambda) + \dots$ 



- Find numerical solutions with no approximations or controllable approximations
- Calculate low-energy observables form the shody wave function and compare with experiment to test nuclear forces and provide predictions when experiments are hard or even not possible or help interpret new experiments
- Develop a strong predictive theory in the framework of light nuclei and then extend it towards heavier and neutron-rich systems



## Ingredients



## **Final State Interaction**

Exact evaluation of the final state in the continuum is limited in energy and A

Solution: The Lorentz Integral Transform Method Efros et al., Nucl.Part.Phys. 34 (2007) R459

Response in the continuum

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

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

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

- Due to imaginary part  $\Gamma$  the solution  $\ket{\psi}$  is unique
- Since the r.h.s. is finite, then  $|\psi
  angle$  has bound state asymptotic behavior

 $L(\sigma, \Gamma)$ 

inversion

 $R(\omega)$  with the exact final state interaction



You can use any good bound state method!

e.g. Hyperspherical Harmonics, No Core Shell Model, Coupled Cluster Theory

March 15 2012

RIUMF

Sonia Bacca

## **Final State Interaction**

Exact evaluation of the final state in the continuum is limited in energy and A

Solution: The Lorentz Integral Transform Method Efros et al., Nucl.Part.Phys. 34 (2007) R459

TRIUMF



March 15 2012

Sonia Bacca

![](_page_6_Picture_0.jpeg)

## **Hyperspherical Harmonics**

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

• Few-body method - uses relative coordinates  $|\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_A)\rangle = |\varphi(\vec{R}_{CM})\Psi(\vec{\eta}_1, \vec{\eta}_2, \dots, \vec{\eta}_{A-1})\rangle$ 

![](_page_6_Picture_5.jpeg)

Recursive definition of hyper-spherical coordinates

, 
$$\Omega$$
  $\rho^2 = \sum_{i=1}^A r_i^2 = \sum_{i=1}^{A-1} \eta_i^2$ 

$$H_0(\rho, \Omega) = T_\rho - \frac{K^2(\Omega)}{\rho^2}$$

 $\rho$ 

$$\Psi = \sum_{[K],\nu}^{K_{max},\nu_{max}} c_{\nu}^{[K]} e^{-\rho/2b} \rho^{n/2} L_{\nu}^{n} (\frac{\rho}{b}) [\mathcal{Y}_{[K]}^{\mu}(\Omega) \chi_{ST}^{\bar{\mu}}]_{JT}^{a}$$

$$\downarrow$$
Asymptotic
$$e^{-a\rho} \quad \rho \to \infty$$

 $K \leq K_{max}$ Matrix Diagonalization

$$\langle \psi | H_{(2)} | \psi \rangle = \frac{A(A-1)}{2} \langle \psi | H_{(A,A-1)} | \psi \rangle$$

Can use local and non-local interactions

Most applications in few-body; challenge in A>4

Barnea and Novoselsky, Ann. Phys. 256 (1997) 192

### 

![](_page_7_Figure_1.jpeg)

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

For the reactions expanding  $~O|\psi_0\rangle$  increase of dimension by at least one order of magnitude of angular momentum is changed

### TRIUMF The LIT with Hyperspherical Harmonics

Numerical example: Dipole Response Function of <sup>4</sup>He  $\hat{O} = \hat{D}_z = \sum (z_i - Z_{cm})$  with NN(N<sup>3</sup>LO) 8  $\Gamma = 10$  MeV K<sub>max</sub> 18  $L \, [fm^2 MeV^{-2} \, 10^{-3}]$ 16 12 10 8  $^{4}\mathrm{He}$ 0 -20 20 40 80 0 60 100 120 σ [MeV]

Inversion of the LIT

Ansatz
$$R(\omega) = \sum_{i}^{I_{\max}} c_{i} \chi_{i}(\omega, \alpha)$$
$$L(\sigma, \Gamma) = \sum_{i}^{I_{\max}} c_{i} \mathcal{L}[\chi_{i}(\omega, \alpha)]$$

Least square fit of the coefficients  $c_i$  to reconstruct the response function

![](_page_8_Figure_5.jpeg)

![](_page_9_Picture_0.jpeg)

### Some examples for A=4

- Photo-absorption
- Electron Scattering

![](_page_10_Figure_0.jpeg)

> Moderate sensitivity to the Hamiltonian used; theory variation about 10% in peak

Sonia Bacca

![](_page_11_Figure_0.jpeg)

 $\Rightarrow$  Moderate sensitivity to the Hamiltonian used; theory variation about 10% in peak

More recent experimental activity seems to confirm higher data with peak around 27 MeV

Theoretical precision is better than experimental error

August 23rd 2012

Sonia Bacca

### ®твимя Inelastic e-Scattering <sup>4</sup>He(e,e')X

![](_page_12_Figure_1.jpeg)

Virtual Photon

 $(\omega, \mathbf{q})$ 

can vary independently

Inclusive cross section A(e,e')X

$$\frac{d^2\sigma}{d\Omega d\omega} = \sigma_M \left[ \frac{Q^4}{\mathbf{q}^4} R_L(\omega, \mathbf{q}) + \left( \frac{Q^2}{2\mathbf{q}^2} + \tan^2 \frac{\theta}{2} \right) R_T(\omega, \mathbf{q}) \right]$$

with  $Q^2 = -q_{\mu}^2 = \mathbf{q}^2 - \omega^2$  and  $\theta$  scattering angle

and  $\sigma_M$  Mott cross section

### ®твимя Inelastic e-Scattering <sup>4</sup>He(e,e')X

![](_page_13_Figure_1.jpeg)

Virtual Photon

 $(\omega, \mathbf{q})$ 

can vary independently

Inclusive cross section A(e,e')X

$$\frac{d^{2}\sigma}{d\Omega d\omega} = \sigma_{M} \left[ \frac{Q^{4}}{\mathbf{q}^{4}} R_{L}(\omega, \mathbf{q}) + \left( \frac{Q^{2}}{2\mathbf{q}^{2}} + \tan^{2} \frac{\theta}{2} \right) R_{T}(\omega, \mathbf{q}) \right]$$

$$\frac{R_{L}(\omega, \mathbf{q})}{f} = \sum_{f} |\langle \Psi_{f} | \rho(\mathbf{q}) | \Psi_{0} \rangle|^{2} \delta \left( E_{f} - E_{0} - \omega + \frac{\mathbf{q}^{2}}{2M} \right) \quad \text{two-body currents are not important}$$

$$R_{T}(\omega, \mathbf{q}) = \sum_{f} |\langle \Psi_{f} | J_{T}(\mathbf{q}) | \Psi_{0} \rangle|^{2} \delta \left( E_{f} - E_{0} - \omega + \frac{\mathbf{q}^{2}}{2M} \right)$$

### RIUMF Inelastic e-Scattering <sup>4</sup>He(e,e')X

### Calculation of $R_L(\omega, \mathbf{q})$ with the LIT

Medium-q kinematics

Searching for 3NF effects

![](_page_14_Figure_4.jpeg)

 $P_{f}^{\boldsymbol{\mu}}$ 

 $P_0^{\mu}$ 

k'"

 $k^{\mu}$ 

 $q^{\mu} = k^{\mu} - k^{\mu}$ 

 $q^{\mu} = (\omega, q)$ 

### RIVMF Inelastic e-Scattering <sup>4</sup>He(e,e')X

![](_page_15_Figure_1.jpeg)

S-DALINAC will maybe take data at lower q

 $P_{f}^{\boldsymbol{\mu}}$ 

 $P_0^{\mu}$ 

k'"

 $k^{\mu}$ 

 $q^{\mu} = k^{\mu} - k^{\mu}$ 

![](_page_16_Figure_1.jpeg)

![](_page_16_Figure_2.jpeg)

![](_page_16_Figure_3.jpeg)

**R**TRIUMF

In proximity of the resonance both in theory and experiment

$$R_{\mathcal{M}}(q,\omega) = R_{\mathcal{M}}^{\mathrm{res}}(q,\omega) + R_{\mathcal{M}}^{\mathrm{bg}}(q,\omega) \quad (\bigstar)$$

We use a square integrable basis (HH) to calculate the LIT (not the response) rigorous because of finite  $\,\Gamma\,$ 

$$\mathcal{L}_{\mathcal{M}}(q,\sigma,\Gamma) = \frac{\Gamma}{\pi} \sum_{\nu=1}^{N} \frac{|\langle \Psi_{\nu} | \mathcal{M}(q) | \Psi_{0} \rangle|^{2}}{(\sigma - e_{\nu} + E_{0})^{2} + \Gamma^{2}}$$

![](_page_17_Figure_5.jpeg)

where  $\Psi_{\nu}, e_{\nu}$  are eigenstate and eigenvalues of H on our basis

We see ONE very pronounced strength  $|\langle \Psi_{\nu_R} | \mathcal{M}(q) | \Psi_0 \rangle|^2$  located at the energy  $e_{\nu} - E_0 = E_R^*$ 

Exploit the power of the LIT method (calculate the far continuum) to subtract the background

 $P_{f}^{\boldsymbol{\mu}}$ 

 $P_0^{\mu}$ 

k'"

In proximity of the resonance both in theory and experiment

 $R_{\mathcal{M}}(q,\omega) = R_{\mathcal{M}}^{\mathrm{res}}(q,\omega) + R_{\mathcal{M}}^{\mathrm{bg}}(q,\omega) \quad (\bigstar)$ 

Inversion of the LIT

ansatz

![](_page_18_Figure_5.jpeg)

least square fit of  $C_i$ 

![](_page_18_Figure_7.jpeg)

k'<sup>µ</sup>

 $\mathbf{k}^{\mu}$ 

 $q^{\mu} = k^{\mu} - k^{\mu}$ 

 $q^{\mu} = (\omega, q)$ 

#### LIT of a delta by $f_R(q)\frac{\Gamma}{\pi}\frac{1}{(\sigma - E_R + E_0)^2 + \Gamma^2}$ numerically choosing

Fit  $f_R(q)$  to obtain a smooth background  $\rightarrow f_R(q)$  is related to the resonant form factor

 $\gamma \ll \Gamma$ 

 $P_{f}^{\boldsymbol{\mu}}$ 

 $P_0^{\mu}$ 

![](_page_19_Figure_1.jpeg)

![](_page_19_Figure_2.jpeg)

**R**TRIUMF

**Resonant Transition Form Factor** 

# RIUMF Sensitivity to Nuclear Hamiltonians

#### S.B. et al., PRL 110, 042503 (2013)

![](_page_20_Figure_2.jpeg)

 $NN(N^{3}LO)+3NF(N^{2}LO) E_{0} = -28.36 MeV$ 

 $E_0^{exp}$ = -28.30 MeV

![](_page_20_Figure_5.jpeg)

## Analysis of this result

Realistic three-nucleon forces do not reproduce the data for  $|F_{\mathcal{M}}|^2$ Particularly large difference are found with chiral EFT potentials. This is unexpected! What can be the source of this behaviour?

• Numerics? Our calculations are well converged (few % level) in the HH basis

K <sub>max</sub>	12	14	16	18

 $10^4 |F_{\mathcal{M}}|^2$  4.59 4.75 4.85 4.87

#### Many-body charge operators?

#### **Conventional Nuclear Physics**

Impulse approximation valid for elastic form factor below 2 fm<sup>-1</sup> Viviani *et al.*, PRL **99** (2007) 112002

#### EFT approach

RIUMF

work done by Park *et al.*, Epelbaum, Koelling *et al.*, Pastore *et al.*, many-body operators appear at high oder in EFT

#### • Higher order 3NF (N<sup>3</sup>LO)? Unlikely...

![](_page_21_Figure_11.jpeg)

![](_page_22_Picture_0.jpeg)

## Analysis of this result

• Location of the resonance?

![](_page_22_Figure_3.jpeg)

The "realistic Hamiltonians" fail to reproduce the correct position of the 0<sup>+</sup><sub>2</sub> resonance

More theoretical work needed to understand this.

• Can this be measured again?

![](_page_23_Picture_0.jpeg)

## One example for A=16

Photo-absorption

#### TRIUMF **Extension to medium-mass nuclei**

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

![](_page_24_Figure_2.jpeg)

 $|\psi_0(\vec{r_1}, \vec{r_2}, ..., \vec{r_A})\rangle = e^T |\phi_0(\vec{r_1}, \vec{r_2}, ..., \vec{r_A})\rangle$ reference SD with any sp states  $T_2$  $T_3$ 

![](_page_24_Figure_4.jpeg)

Friday, 19 April, 13

## **Extension to medium-mass nuclei**

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

![](_page_25_Figure_2.jpeg)

R. Roth et al., Phys. Rev. Lett. 109, 052501 (2012)

LIT+CC can possibly extend calculations of inelastic reactions into medium-mass nuclei!

What about electro-weak reactions?

#### RIUMF

## LIT with Coupled Cluster Theory

![](_page_26_Picture_2.jpeg)

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

S.B., N.Barnea, G.Hagen, G.Orlandini, T.Papenbrock, arXiv:1303.7446

$$\begin{split} L(\sigma,\Gamma) &= \left\langle \tilde{\Psi} | \tilde{\Psi} \right\rangle \longrightarrow \left\langle \tilde{\Psi}_L | \tilde{\Psi}_R \right\rangle = \left\langle \Phi_0 \hat{L}(z) | \hat{R}(z^*) \Phi_0 \right\rangle \quad \text{with} \quad z = E_0 + \sigma + i\Gamma \\ \hat{R}_0 + \sum_{ia} \hat{R}_i^a \hat{c}_a^\dagger \hat{c}_i + \frac{1}{4} \sum_{ijab} \hat{R}_{ij}^{ab} \hat{c}_a^\dagger \hat{c}_b^\dagger \hat{c}_j \hat{c}_i + \dots \\ \hat{L}_0 + \sum_{ia} \hat{L}_i^a \hat{c}_i^\dagger \hat{c}_a + \frac{1}{4} \sum_{ijab} \hat{L}_{ij}^{ab} \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_b \hat{c}_a + \dots \end{split}$$

i ne Schrödinger-like eq. becomes

$$\begin{split} & \tilde{|\Psi_R\rangle} \\ & (\bar{H} - z^*)\hat{R}(z^*)|\Phi_0\rangle = \bar{\Theta}|\Phi_0\rangle \quad \text{with} \quad \bar{\Theta} = e^{-T}\Theta e^T \quad \text{similarity transformed operator} \\ & \hat{R}(z^*)\bar{H}|\Phi_0\rangle = E_0\hat{R}(z^*)|\Phi_0\rangle \\ & [\bar{H},\hat{R}(z^*)]|\Phi_0\rangle = (z^* - E_0)\hat{R}(z^*)|\Phi_0\rangle + \bar{\Theta}|\Phi_0\rangle \quad \text{Right EoM to find the amplitudes of } \hat{R} \\ & \langle \Phi_0|[\hat{L}(z),\bar{H}] = \langle \Phi_0|\hat{L}(z)(z - E_0) + \langle \Phi_0|\bar{\Theta}^{\dagger} & \text{Right EoM to find the amplitudes of } \hat{L} \end{split}$$

![](_page_27_Picture_0.jpeg)

![](_page_27_Picture_2.jpeg)

**Dipole Response Function** 

S.B., N.Barnea, G.Hagen, G.Orlandini, T.Papenbrock, arXiv:1303.7446

Validation on <sup>4</sup>He with NN forces derived from  $\chi$ EFT (N<sup>3</sup>LO)

![](_page_27_Figure_6.jpeg)

Convergence in the model space expansion

![](_page_27_Figure_8.jpeg)

![](_page_28_Picture_0.jpeg)

![](_page_28_Figure_1.jpeg)

The comparison with exact theory is very good!

![](_page_29_Picture_1.jpeg)

**Dipole Response Function** 

S.B., N.Barnea, G.Hagen, G.Orlandini, T.Papenbrock, arXiv:1303.7446

Extension to <sup>16</sup>O with NN forces derived from  $\chi$ EFT (N<sup>3</sup>LO)

TRIUMF

Convergence in the model space expansion

![](_page_29_Figure_7.jpeg)

![](_page_30_Picture_0.jpeg)

![](_page_30_Picture_2.jpeg)

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

S.B., N.Barnea, G.Hagen, G.Orlandini, T.Papenbrock, <u>arXiv:1303.7446</u>

#### Extension to <sup>16</sup>O with NN forces derived from $\chi$ EFT (N<sup>3</sup>LO)

![](_page_30_Figure_6.jpeg)

Comparison with experiment

![](_page_30_Figure_8.jpeg)

Data: target absorption experiment with  $\gamma$ 

![](_page_30_Picture_10.jpeg)

Sonia Bacca

![](_page_31_Picture_0.jpeg)

![](_page_31_Picture_2.jpeg)

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

S.B., N.Barnea, G.Hagen, G.Orlandini, T.Papenbrock, arXiv:1303.7446

#### Extension to <sup>16</sup>O with NN forces derived from $\chi$ EFT (N<sup>3</sup>LO)

![](_page_31_Figure_6.jpeg)

Comparison with experiment

![](_page_31_Figure_8.jpeg)

![](_page_32_Picture_0.jpeg)

## **Conclusions and Outlook**

- Nuclear response functions are very rich observables to test our understanding on nuclear forces
- Extending these calculations to medium mass nuclei is possible and very exciting

### **Perspectives**

- Dipole response function in <sup>40</sup>Ca, <sup>48</sup>Ca, electric dipole polarizability Dipole response function of neutron-rich Oxygen isotope
- Quadrupole or monopole excitation of medium mass nuclei
   need extension of LIT/CCSD to two-body operator
- Magnetic transitions for medium mass nuclei with two-body currents
   need extension of LIT/CCSD to two-body operator
- Add triples and three-nucleon forces

![](_page_33_Picture_0.jpeg)

### Thanks to my collaborators

![](_page_33_Picture_2.jpeg)

Nir Barnea, Doron Gazit

![](_page_33_Picture_4.jpeg)

Gaute Hagen, Thomas Papenbrock

![](_page_33_Picture_6.jpeg)

Winfried Leidemann, Giuseppina Orlandini

## Thank you!