Nuclear Struclear Structure and Reactions: Experimental and Ab-Initio Perspetives TRIUMF, 18-21 February 2014

## Ab-Initio Studies of Three-Body Interactions around O and Ca isotopes

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## Outilne:

- Dyson (closed-shell) and Gorkov (open shells) formalisms of GF
- Inclusion of 3 NF and fluorine/nitrogen driplines
- Spectral functions and masses around ${ }^{A} \mathrm{O}$ and ${ }^{A} \mathrm{Ca}$
- Applications of SCGF to reactions-optical models
V. Somà, A. Cipollone, CB, P. Navrátil, T. Duguet, arXiv:1312.2068 [nucl-th]
A. Carbone, A. Cipollone, CB, A. Rios, A. Polls, Phys. Rev. C88, 054326 (2013)
A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. 111, 062501 (2013)
V. Somà, CB, and T. Duguet, , arXiv:1311.1989 [nucl-th] - Phys. Rev C, in print
V. Somà, CB, and T. Duguet, Phys. Rev. C 87, 011303R (2013)
V. Somà, T. Duguet, and CB, Phys. Rev. C 84, 064317 (2011)


## Green's functions in many-body theory

One-body Green's function (or propagator) describes the motion of quasiparticles and holes:

$$
g_{\alpha \beta}(E)=\sum_{n} \frac{\left\langle\Psi_{0}^{A}\right| c_{\alpha}\left|\Psi_{n}^{A+1}\right\rangle\left\langle\Psi_{n}^{A+1}\right| c_{\beta}^{\dagger}\left|\Psi_{0}^{A}\right\rangle}{E-\left(E_{n}^{A+1}-E_{0}^{A}\right)+i \eta}+\sum_{k} \frac{\left\langle\Psi_{0}^{A}\right| c_{\beta}^{\dagger}\left|\Psi_{k}^{A-1}\right\rangle\left\langle\Psi_{k}^{A-1}\right| c_{\alpha}\left|\Psi_{0}^{A}\right\rangle}{E-\left(E_{0}^{A}-E_{k}^{A-1}\right)-i \eta}
$$

...this contains all the structure information probed by nucleon transfer (spectral function):


## Faddeev-RPA in two words...

## Self-energy (optical potential):



Phys.Rev.C63,

- A complete expansion requires all types of particle-vibration coupling: $\checkmark \quad g^{\text {II }}(\omega) \rightarrow$ pairing effects, two-nucleon transfer $\checkmark \Pi^{(\mathrm{ph})}(\omega) \rightarrow$ collective motion, using RPA or beyond
$\checkmark$ Pauli exchange effects
- The Self-energy $\Sigma^{\star}(\omega)$ yields both single-particle states and scattering
- Finite nuclei: $\rightarrow$ require high-performance computing


## Faddeev-RPA in two words...

Particle vibration coupling is the main cause driving the distribution of particle strength-a least close to the Fermi surface...


## Open－shells： $1^{\text {st }} \& 2^{\text {nd }}$ order Gorkov diagrams

V．Somà，CB，T．Duguet，，arXiv：1311．1989［nucl－th］－PRC，in print
V．Somà，CB，T．Duguet，Phys．Rev．C 87，011303R（2013）
V．Somà，T．Duguet，CB，Phys．Rev．C 84， 064317 （2011）
粦 $1^{\text {st }}$ order $" \rightarrow$ energy－independent self－energy


粦 $2^{\text {nd }}$ order $" \rightarrow$ energy－dependent self－energy

$$
\Sigma_{a b}^{11(2)}(\omega)={ }_{c}^{a} \omega_{d}^{d} d_{b}^{a}
$$

粦 Gorkov equations
$\longrightarrow$ eigenvalue problem

$$
\left.\sum_{b}\left(\begin{array}{cc}
t_{a b}-\mu_{a b}+\Sigma_{a b}^{11}(\omega) & \Sigma_{a b}^{12}(\omega) \\
\Sigma_{a b}^{21}(\omega) & -t_{a b}+\mu_{a b}+\Sigma_{a b}^{22}(\omega)
\end{array}\right)\right|_{\omega_{k}}\binom{\mathcal{U}_{b}^{k}}{\mathcal{V}_{b}^{k}}=\omega_{k}\binom{\mathcal{U}_{a}^{k}}{\mathcal{V}_{a}^{k}}
$$

$$
\begin{aligned}
\mathcal{U}_{a}^{k *} & \equiv\left\langle\Psi_{k}\right| \bar{a}_{a}^{\dagger}\left|\Psi_{0}\right\rangle \\
\mathcal{V}_{a}^{k *} & \equiv\left\langle\Psi_{k}\right| a_{a}\left|\Psi_{0}\right\rangle
\end{aligned}
$$

V. SOMA, T. DUGUET, AND C. bARBIERI PHYSICAL REVIEW C 84, 064317 (2011)

Espressions for $1^{\text {st }} \& 2^{\text {nd }}$ order diagrams


Ab INITIO SELECONSISTENT GORKOV-GREEN's
5. Block-diagonal structu
a. First ord
ck-diagona

The goal of this subsection is to discuss how the block-idagonona
reffects in the various self-energy contributions, starting with the fir reflects in the various self-energy contributions, starting and (C19) into Eq. (B7), and introducing the factor

$$
f_{\alpha \beta, y^{n}, n, n_{n}}^{n_{n}, \delta_{a p} \delta_{n, n}}
$$

one obtains
$\Sigma_{a b}^{1(1)}=\sum_{c, i, k} V_{\text {atid }} D_{d}^{+} D_{c}^{k}$



$$
\equiv \delta_{u p} \delta_{n, \ldots, m} \Sigma_{n, 0}^{11(a)(1)}
$$

$\equiv \delta_{u p} \delta_{n, \ldots,}, \Lambda_{n, n_{2}}^{a l}$,
here the block-diagonal normal density matrix is introduced throu



$$
\Sigma_{a b}^{22(1)}=-\sum_{c d, k} v_{b s a d} \bar{v}_{c}^{+} \bar{\nu}_{d}^{*}
$$

$=-\delta_{a p} \delta_{n, \omega_{0}} \sum_{k \times n_{i}} \sum_{\gamma} \sum_{j} f_{a y}^{n_{i}}$
$\equiv \delta_{0, p} \delta_{m_{0}, x_{8}}, \Sigma_{n, t)}^{2[a \mid(1)}$


Let us o
derives

$$
\Sigma_{a b}^{12(1)}=\frac{1}{2} \sum_{c d, k} v_{a b e d} \nu_{c}^{k} \cdot \bar{u}_{d}^{k}
$$


$=-\frac{1}{2} \sum_{n, s e} \sum_{V} \sum_{m_{i}} \sum_{j} f_{\text {wipry }}^{\operatorname{ceven}} \eta_{b} \eta_{b} \eta_{c} C_{j=}^{j 0}$


$\equiv \delta_{a p} \delta_{n, 0, w}, \Sigma_{n, n}^{12[|a|(a)}$
$\equiv \delta_{a \beta} \delta_{\operatorname{cosen}} \hat{h}_{n, n}^{(\alpha)}$,
V. SOMÃ, T. DUGUET, AND C. BARBIERI

It is interesting to note that the first-order a with a $J=0$ many-body state. The other:

$$
\begin{aligned}
& \Sigma_{a b}^{21(1)}=\frac{1}{2} \sum_{c j, k} \bar{v}_{\text {cab }} \overline{\mathcal{U}} \\
& =-\frac{1}{2} \sum_{n, N \sim 0} \sum_{\gamma} \\
& =\delta_{a s} \delta_{n=0, m}, \frac{1}{2} \\
& \equiv \delta_{a p} \delta_{r e . . . .}, \Sigma_{n_{0}}^{21} \\
& =\delta_{a p} \delta_{n, 0, m}, \hbar_{n o l}^{[\alpha]}
\end{aligned}
$$

Block-diagonal forms of second-order s angular momentum couplings of the three $\mathcal{Q}, \mathcal{R}$, and $\mathcal{S}$. One proceeds first coupling give $J_{\text {uce }}$. The recoupled $\mathcal{M}$ term is compu


$=\sum_{M_{1} W_{2} w_{j}, M_{c}} \sum_{m} \sum_{j, M_{c}} \delta_{x_{1}, \rho} \delta_{m_{2},}$,





where general properties of Clebsch-Gord
$\equiv \delta_{S_{m i} / \delta} \delta_{M_{m} m_{\sim}} \mathcal{N}_{n}$
One can show that the same result is obtai





## 064317-29

These terms are finally put together to form the different contributions to second-order self-energies. Let us consider $\Sigma^{11(z)}$ as an example [sec Eq. (75)]. By inserting Eqs. (C35) and (C36) and summing over all possible total and intermediate angular momenta, one has
(C37)
which recovers relation (72a). The remaining quantities [see Eqs. (69) and (70)] are related to $\mathcal{M}$ and $\mathcal{N}$ by permutations of $\left\{k_{1}, k_{2}, k_{3}\right\}$ indioes and can be obtained from Eqs. (C35) and (C36) by taking into account the different recoupling of $j_{k}, j_{2}$ and $j_{k}$, to $J_{\text {ixe }}$ and $J_{c}$ as follows
(C38)



${ }_{4}^{1}\left(\omega^{\prime}\right) G_{g^{\prime \prime}}^{11}\left(\omega^{\prime \prime}\right) G_{\xi^{\prime \prime}}^{\prime \prime}\left(\omega^{\prime}+\omega^{\prime \prime}-\omega\right)$


C41)

## Approaches in GF theory

| Truncation <br> scheme: | Dyson formulation <br> (closed shells) | Gorkov formulation <br> (semi-magic) |
| :--- | :---: | :---: |
| $1^{\text {st }}$ order: | Hartree-Fock | HF-Bogolioubov |
| $2^{\text {nd }}$ order: | $2^{\text {nd }}$ order | $2^{\text {nd }}$ order (w/ pairing) |
| $\ldots$ | $\ldots$ |  |
| $3^{\text {rd }}$ and all-orders <br> sums, <br> P-V coupling: | ADC(3) | FRPA |

## Approaches in GF theory



## Modern realistic nuclear forces

Chiral EFT for nuclear forces:

(3NFs arise naturally at N2LO)

|  | 2 N forces $\quad 3 \mathrm{~N}$ forces | 4 N forces |
| :---: | :---: | :---: |
| $\mathrm{LO} \mathcal{O}\left(\frac{Q^{0}}{\Lambda^{0}}\right)$ | $\gamma / \quad\|-\cdots\|$ |  |
| $\mathrm{NLO} \mathcal{O}\left(\frac{Q^{2}}{\Lambda^{2}}\right)$ |   | —— |
| $\mathrm{N}^{2} \mathrm{LO} \mathcal{O}\left(\frac{Q^{3}}{\Lambda^{3}}\right)$ |  |  |
| $\mathrm{N}^{3} \mathrm{LO} \mathcal{O}\left(\frac{Q^{4}}{\Lambda^{4}}\right)$ |  |  $+$ |

Single particle spectrum at $E_{\text {fermi }}$ :

[T. Otsuka et al.
Phys Rev. Lett 105, 32501 (2010)]

Need at LEAST 3NF!!!
("cannot" do RNB physics without...)

Saturation of nuclear matter:


## Chiral Nucler forces SRG evolved



## Inclusion of NNN forces

A. Carbone, CB, et al., Phys. Rev. C88, 054326 (2013)

粦 NNN forces can enter diagrams in three different ways:


Correction to external 1-Body interaction


Correction to non-contracted 2-Body interaction

- Contractions are with fully correlated density matrices (BEYOND a normal ordering...)



## Inclusion of NNN forces

A. Carbone, CB, et al., Phys. Rev. C88, 054326 (2013)

粦 NNN forces can enter diagrams in three different ways:
$\rightarrow$ Define new 1- and 2-body interactions and use only interaction-irreducible diagrams

$$
\begin{aligned}
& \tilde{U}=\cdots x \equiv \cdots+\frac{1}{4} \equiv \cdots+\cdots \cdots \\
& \tilde{V}=\cdots \cdots \cdots \\
& W=\cdots \cdots \cdots \cdots \cdots
\end{aligned}
$$

- Contractions are with fully correlated density matrices (BEYOND a normal ordering...)


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$$
\begin{aligned}
& \left.\tilde{\mathrm{U}}=\sum_{\alpha \beta}\left[-U_{\alpha, \beta}-\mathrm{i} \hbar \sum_{\gamma \delta} V_{\alpha \gamma, \beta \delta}\right) G_{\delta \gamma}\left(t-t^{+}\right)+\frac{\mathrm{i} \hbar}{4} \sum_{\substack{\gamma \epsilon \\
\delta \eta}} W_{\alpha \gamma \epsilon, \beta \delta \eta} G_{\delta \eta, \gamma \epsilon}^{I I}\left(t-t^{+}\right)\right] a_{\alpha}^{\dagger} a_{\beta} \\
& \tilde{V}=\frac{1}{4} \sum_{\substack{\alpha \gamma \\
\beta \delta}}\left[V_{\alpha \gamma, \beta \delta}-\mathrm{i} \hbar \sum_{\epsilon \eta} W_{\alpha \gamma \epsilon, \beta \delta \eta} G_{\eta \epsilon}\left(t-t^{+}\right)\right] a_{\alpha}^{\dagger} a_{\gamma}^{\dagger} a_{\delta} a_{\beta} \\
& \mathbf{W}=\cdots
\end{aligned}
$$

- Contractions are with fully correlated density matrices (BEYOND a normal ordering...)


## NNN forces in FRPA/FTDA formalism

A. Cipollone, CB
$\rightarrow$ Ladder contributions to static self-energy are negligible (in oxygen)


## Inclusion of NNN forces

A. Carbone, CB, et al., Phys. Rev. C88, 054326 (2013)

- Second order PT diagrams with 3BFs: effectively:


FIG. 4. The one interaction irreducible diagrams (a) and the three interaction reducible ones (b, c and d) that are contained in Fig. 3a.

## Inclusion of NNN forces

A. Carbone, CB, et al., Phys. Rev. C88, 054326 (2013)

- Second order PT diagrams with 3BFs:

(a)

(b)
- Third order PT diagrams with 3BFs:

(n)

(b)

(f)





## Inclusion of NNN forces

A. Carbone, CB, et al., Phys. Rev. C88, 054326 (2013)

- Third ondenPT diagrams with 3BFs:
- Second order PT diagrams with 3BFs:

(a)

(b)



## Results for the $\mathrm{N}-\mathrm{O}-\mathrm{F}$ chains

A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. 111, 062501 (2013)


$\rightarrow$ 3NF crucial for reproducing binding energies and driplines around oxygen
$\rightarrow$ d3/2 raised by genuine 3NF
$\rightarrow$ cf. microscopic shell model [Otsuka et al, PRL105, 032501 (2010).]

N3LO ( $\Lambda=500 \mathrm{Mev} / \mathrm{c}$ ) chiral NN interaction evolved to $2 \mathrm{~N}+3 \mathrm{~N}$ forces $\left(2.0 \mathrm{fm}^{-1}\right.$ ) N2LO $(\Lambda=400 \mathrm{Mev} / \mathrm{c})$ chiral 3N interaction evolved $\left(2.0 \mathrm{fm}^{-1}\right)$

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## Neutron spectral function of Oxygens



## Calcium isotopic chain

Ab-initio calculation of the whole Ca chain with NN+3N forces

$\rightarrow$ induced and full3NF investigated
$\rightarrow$ genuine (N2LO) 3NF needed to correct the energy curvature
$\rightarrow$ Full 3NF give a correct trend but overbind!
$\rightarrow$ convergence worsens after $A \approx 52$

## Calcium isotopic chain

Ab-initio calculation of the whole Ca chain with $\mathrm{NN}+3 \mathrm{~N}$ forces

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$\rightarrow$ Full 3NF give a correct trend but overbind!
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## Calcium isotopic chain

Two-neutron separation energies

$\rightarrow$ induced and full3NF investigated
$\rightarrow$ genuine (N2LO) 3NF needed to reproduce $\mathrm{S}_{2 n}$
$\rightarrow \mathrm{N}=20$ and $\mathrm{Z}=20$ gaps overestimated!

## Neighbouring chains: Ar, K, Sc, Ti <br> V. Somà, CB et al., arXiv:1312.2068 [nucl-th]



$\rightarrow$ induced and full3NF investigated
$\rightarrow$ genuine (N2LO) 3NF needed to reproduce $S_{2 n}$
$\rightarrow \mathrm{N}=20$ and $\mathrm{Z}=20$ gaps overestimated!

Optical Potentials Based on the Nuclear Self-energy

## Self-Consistent Green's Function Approach

optical potential
[CB, Jennings, Nucl. Phys A758, 395c (2005)
Phys Rev. C72, 014613 (2005)]


## Nucleon elastic scattering



The irreducible self-energy is a nucleon-nucleus optical potential [see e.g. Mahaux and Sartor, Adv. Nucl. Phys. 20, (1991)]

$$
\Sigma^{\star}\left(\mathbf{r}, \mathbf{r}^{\prime} ; \varepsilon\right)=\Sigma_{\alpha \beta}^{H F}-\frac{1}{\pi} \int_{\text {mean-field }}^{\infty} d E^{\prime} \frac{\operatorname{Im} \Sigma^{\star}\left(\mathbf{r}, \mathbf{r}^{\prime} ; E^{\prime}\right)}{\varepsilon-E^{\prime}+i \eta}, \underbrace{+\frac{1}{\pi} \int_{-\infty}^{\varepsilon_{T}^{\zeta}} d E^{\prime} \frac{\operatorname{Im} \Sigma^{\star}\left(\mathbf{r}, \mathbf{r}^{\prime} ; E^{\prime}\right)}{\varepsilon-E^{\prime}-i \eta}}_{\begin{array}{l}
\text { resonances } \\
\text { beyond mean-field }
\end{array}}
$$

$\rightarrow$ This provides consistent overlaps and scattering A-1 wave functions

## p-16O phase shifts - positive parity waves

[C.B., B.Jennings,


Phys. Rev. C72, 014613 (2005)]
-AV18 interaction
-The phase shift are in agreement with the experiment!
-BUT does not reproduce phase shifts and bound state energies at the same time
$\rightarrow$ need for improved H / 3NF
-Non-MF resonances "OK"

## Convergence of Ab-Initio Calculated Optical Potentials

- $J_{w}$ : integral over the imaginary optical potential (overall absorption)
- angular momentum dependence (non locality) not negligible!
$\rightarrow$ in particular below $E_{F}$

S. Waldecker, CB, W.Dickhoff - Phys. Rev. C84, 034616 (2011)


## Correlations in sp energies and strengths



## Microscopic Optical Potential from FRPA

- absorption away from $E_{F}$ is enhanced by the tensor force
- little effects from charge exchange (e.g. p-48 $\mathrm{Ca}<->\mathrm{n}-{ }^{48} \mathrm{Sc}$ )


$J_{w}$ : integral over the imaginary opt. pot (overall absorption)

| $\ldots \ldots$ Full FRPA result (w/ av18) |  |
| :--- | :--- |
| Charge-exchange d.o.f. suppressed |  |
|  | Tensor force suppressed |

## Collaborators



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## Conclusions

- The GORKOV formulation permits for the first time ab-initio calculations of binding energies, spectral quantities, and so on... for open-shell semi-magic nuclei: this means MANY of THEM, in the MID-MASS region, and previously out of reach for ab-initio.
- Consistent prediction of s.p, spectral distribution and scattering
- Performance of chiral nuclear forces for finite nuclei:
- Leading three nucleon forces (NNLO) are ALWAYS needed to explain the proper trends. They equally set the driplines of $O, N$, and $F$.
- N, O, F region: binding energies are predicted OK ( $\leqslant 1 \%$ ) radii small.
- Ar, K, Ca, Sc, Ti region: overbound by $\sim 1 \mathrm{MeV} / \mathrm{A}$.
- $N=20, Z=20$ gaps and separations among major shells are exaggerated.
- Absorption in optical potentials above the girant resonances dominated by tensor force.



## Evolved chiral 3NF and the Ca isotopes

A. Cipollone, CB, V.Somà, P. Navratil


N3LO ( $\Lambda=500 \mathrm{Mev} / \mathrm{c}$ ) chiral NN interaction evolved to $2 \mathrm{~N}+3 \mathrm{~N}$ forces $\left(2.0 \mathrm{fm}^{-1}\right)$ N2LO $(\Lambda=400 \mathrm{Mev} / \mathrm{c})$ chiral 3 N interaction evolved $\left(2.0 \mathrm{fm}^{-1}\right)$

# Single nucleon transfer in the oxygen chain 

[F. Flavigny et al, PRL110, 122503 (2013)]
$\rightarrow$ Analysis of ${ }^{14} \mathrm{O}(\mathrm{d}, \mathrm{t})^{13} \mathrm{O}$ and ${ }^{14} \mathrm{O}\left(\mathrm{d},{ }^{3} \mathrm{He}\right)^{13} \mathrm{~N}$ transfer reactions @ SPIRAL





- Overlap functions and strengths from GF
- Rs independent of asymetry

