Progress in Ab-Initio Techniques in Nuclear Physics

## Evolution of correlations and shell model charges from SCGF

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Collaborators:
A. Cipollone, CB, P. Navrátil:

Phys. Rev. Lett. 111, 062501 (2013) arXiv:1412.0491 [nucl-th] (2014)
V. Somà, A. Cipollone, CB, P. Navrátil, T. Duguet: Phys.Rev. C 89, $061301 R$ (2014)

CB, J. Phys.: Conf. Ser. 529, 012005 (2014)

## Nuclear forces in exotic nuclei

Nucleon interactions are very complex and difficult to handle

## Change of regime from stable to dripline isotopes !



Neutron-rich matter ( $\mathrm{N}>\mathrm{Z}$ ):

- Neutron star matter EoS
- Symmetry energy

Driplines of nitrogen and fluorine isotopes
Three-nucleon Force (3NF)
[A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. 111, 062501 (2013)]

Tensor force (p-n)


## Example of spectral function ${ }^{56} \mathrm{Ni}$

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):


## Concept of correlations

independent particle, picture

Spectral function: distribution of momentum ( $\mathrm{p}_{\mathrm{m}}$ ) and energies ( $\mathrm{E}_{\mathrm{m}}$ )

[CB and W. H. Dickhoff, Prog. Part. Nucl. Phys 52, 377 (2004)]

## Concept of correlations

independent particle picture

Spectral function: distribution of momentum ( $\mathrm{p}_{\mathrm{m}}$ ) and

Particle-vibration

## $\overline{==-\square}$

 So far, fully characterised only fo rs...!stable
[W. Dickhoff, CB, prog. Part. Null. Phys. $52,377(2004)$ ]

$$
\begin{equation*}
100-150 \tag{2004}
\end{equation*}
$$


[Mougey et al., Nucl. Phys. A335, 35 (1980)]
[CB and W. H. Dickhoff, Prog. Part. Nucl. Phys 52, 377 (2004)]

| 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) <br> FRPA | G-ADC(3) |

## Approaches in GF theory



## Gorkov self-energy up to 2nd order

 V . SOMÃ, T. DUGUET, AND C. BARBIERI

Ab LNITIO SELR:CONSISTENT GORKOV-GREEN's,
5. Block-diagonal structu
a. First ord
ck-diagona

The goal of this subsection is to discuss how the block-diagona
reflects in the various self-energy contributions, starting with the fin reflicets in the various self-energy contributions, star

$$
f_{a \beta, y^{n}, n_{0},}^{n} \equiv \sqrt{1+\delta_{a p} \delta_{n, n}}
$$

one obtains
$\Sigma_{a b}^{1(1)}=\sum_{c, i, k} \nabla_{a t a d} D_{d}^{+} \nu_{c}^{t}$


$\equiv \delta_{a p} \delta_{n, m,} \Sigma_{n, 0}^{11(1)(1)}$
$\equiv \delta_{a \rho} \delta_{n, m_{0},}, \Lambda_{n, n_{p},}^{(a)}$.
where the block-diagonal normal density matrix is introduced throu
and properties of Clebsch-Gocdan coefficients has been used. The $\delta_{\pi, \pi}$, and $\delta_{q, 9}$, leading to $\delta_{\text {of }}=\delta_{l, \delta_{0}} \delta_{\pi, \pi,} \delta_{q, a}$. Similarly, for $\Sigma^{22(1}$

Let us consider the anomalous contributions to the first-order self-en derives

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


$=\sum_{m_{1}, w_{2}, M_{1}, M_{r}} \sum_{j=1} \sum_{\delta_{1}, \rho} \delta_{m_{0},}$





where general properties of Clebsch-Gord
$\equiv \delta_{S_{w} j_{\alpha}} \delta_{M_{m u} m_{\sim}} \mathcal{N}_{n}$
One can show that the same result is obta



These terms are finally put together to form dhe diet an example [see Eq. (75)]. By inserting Eqs. (C35) and (C36) and summing over all possible total and intermediate angular momenta, one has
(C48a)




#  

## 6. Block-diagonal structure of Gorkor's equations

$$
\text { introducing block-diagonal forms for amplitudes } \mathcal{W} \text { and } \mathcal{Z} \text { through }
$$

 ..... (C46a)
with



$$
\begin{aligned}
& \mathcal{R}_{a\left(J_{t} L_{\omega}\right)}^{k_{k} k_{j}}=\sum_{J_{f}}(-1)^{2 \lambda^{2}+2 J_{J}} \sqrt{2 J_{\varepsilon}+1}
\end{aligned}
$$

$$
\begin{aligned}
& \Sigma_{a b}^{12(1)}=\frac{1}{2} \sum_{c d, k} \nu_{a k e d} \nu_{c}^{k} \cdot \vec{u}_{\sigma}^{k}
\end{aligned}
$$

$\equiv \delta_{a p} \delta_{n, c_{0},} \Sigma_{n, n+n}^{12[\mid] \mid(1)}$
$\equiv \delta_{\alpha \beta} \delta_{n, \ldots, m} \hat{h}_{n, n}^{(\alpha)}$,

$$
\begin{align*}
& \Sigma_{c b}^{22(1)}=-\sum_{c d, k} v_{b c o d} \bar{v}_{c}^{*} \bar{\nu}_{d}^{*} . \\
& =-\delta_{a p} \delta_{n, w_{j}} \sum_{n \in m} \sum_{\gamma} \sum_{J} f_{a \gamma}^{m_{i}} \\
& \equiv \delta_{0 p} \delta_{m_{0}, m_{0}} \Sigma_{n, 0}^{2[1](1)} \\
& =-\delta_{a p} \delta_{r_{0}, m_{0}} \Lambda_{n, \Lambda_{0}}^{[q]} \\
& =-\delta_{a \beta} \delta_{\delta_{n, t a s}}\left[\Lambda_{n, \alpha_{0}}^{(a)}\right]^{*} \text {. } \tag{480}
\end{align*}
$$

## Gorkov self-energy up to 2nd order

V. Somà, CB, T. Duguet, , Phys. Rev. C 89, 024323 (2014)
$1^{\text {st }}$ order $" \rightarrow$ energy-independent
V. Somà, CB, T. Duguet, Phys. Rev. C 87, 011303R (2013)
V. Somà, T. Duguet, CB, Phys. Rev. C 84, 064317 (2011) self-energy

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


$$
\Sigma_{a b}^{12(2)}(\omega)=
$$



## The FRPA Method in Two Words

Particle vibration coupling is the main cause driving the distribution of particle strength-on both sides of the Fermi surface...

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CB et al.,
Phys. Rev. C63, 034313 (2001)
Phys. Rev. A76, 052503 (2007)
Phys. Rev. C79, 064313 (2009)
```

- A complete expansion requires all types of particle-vibration coupling
...these modes are all resummed exactly and to all orders in a ab-initio many-body expansion.
-The Self-energy $\Sigma^{\star}(\omega)$ yields both single-particle states and scattering



## Ab-initio Nuclear Computation \& BcDor code

BoccaDorata code:
(C. Barbieri 2006-14
V. Somà 2011-14
A. Cipollone 2012-13)

- Provides a C++ class library for handling many-body propagators ( $\approx 40,000$ lines, OpenMPI based).
- Allows to solve for nuclear spectral functions, many-body propagators, RPA responses, coupled cluster equations and effective interaction/charges for the shell model.

Code history:

core functions and FRPA shell model charges-interactions (lowest order) new Gorkov formalism for open-shell nuclei (at $2^{\text {nd }}$ order)

Coupled clusters equations
Three-nucleon forces ( $\approx 50$ cores, 35 Gb but on the rise...)

Gorkov at $3^{\text {rd }}$ order (will become massively parallel...)

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## Quenching of absolute spectroscopic factors

[CB, Phys. Rev. Lett. 103, 202520 (2009)]

Overall quenching of spectroscopic factors is driven by:
SRC $\quad \rightarrow$ ~10\% part-vibr. coupling $\rightarrow$ dominant "shell-model" $\rightarrow$ in open shell

... with analogous conclusions for ${ }^{48} \mathrm{Ca}$

|  | 10 osc. shells |  |  | Exp. [30] | $1 p 0 f$ space |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | FRPA <br> (SRC) | full <br> FRPA | $\begin{aligned} & \text { FRPA } \\ & +\Delta Z_{\alpha} \end{aligned}$ |  | FRPA | SM | $\Delta Z_{\alpha}$ |
| $\left\{\begin{array}{l} { }^{57} \mathrm{Ni}: \\ v 1 p_{1 / 2} \end{array}\right.$ | 0.96 | 0.63 | 0.61 |  | 0.79 | 0.77 | -0.02 |
| $v 0 f_{5 / 2}$ | 0.95 | 0.59 | 0.55 |  | 0.79 | 0.75 | -0.04 |
| $v 1 p_{3 / 2}$ | 0.95 | 0.65 | 0.62 | $0.58(11)$ | 0.82 | 0.79 | -0.03 |
| $\begin{aligned} & { }^{55} \mathrm{Ni}: \\ & v 0 f_{7 / 2} \end{aligned}$ | 0.95 | $0.72$ | $0.69$ |  | $0.89$ | $0.86$ | -0.03 |

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## Reaching medium mass and neutron rich isotopes

$\rightarrow$ Degenerate system (open shells, deformations...)
$\rightarrow$ Hamiltoninan, including three nucleon forces


## Convergence of s.p. spectra w.r.t. SRG

Cutoff dependence is reduces, indicating good convergence of many-body truncation and many-body forces


NN terms (no induced 3NF) $\leftarrow \rightarrow N N+3 N F$ fully included

## Results for the N-O-F chains

A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. 111, 062501 (2013) and arXiv:1412.0491 [nucl-th] (2014)


## Results for the N-O-F chains

A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. 111, 062501 (2013) and arXiv:1412.0491 [nucl-th] (2014)

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

## Results for the oxygen chain

A. Cipollone, CB, P. Navrátil, arXiv:1412.0491 [nucl-th] (2014)

$\rightarrow$ Single particle spectra slightly diluted and
$\rightarrow$ systematic underestimation of radii

## The sd-pf shell gap

Neutron spectral distributions for ${ }^{48} \mathrm{Ca}$ and ${ }^{56} \mathrm{Ni}$ :
$2 N+3 N F$ (induced)

$2 N+3 N F(F U L L)$


- sd-pf separation is overestimated even with leading order N2LO 3NF
- Correct increase of $p_{3 / 2}-f_{7 / 2}$ splitting (see Zuker 2003)

CB et al., arXiv:1211.3315 [nucl-th]

|  | 2NF only | 2+3NF(ind.) | 2+3NF(full) | Experiment |
| ---: | :---: | :---: | :---: | :---: |
| ${ }^{16} \mathrm{O}:$ | 2.10 | 2.41 | 2.38 | $2.718 \pm 0.210[19]$ |
| ${ }^{44} \mathrm{Ca}:$ | 2.48 | 2.93 | 2.94 | $3.520 \pm 0.005[20]$ |

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## Neutron spectral function of Oxygens



Suncrive

## Z/N asymmetry dependence of SFs - Theory

Ab-initio calculations explain the $\mathrm{Z} / \mathrm{N}$ dependence but the effect is much lower than suggested by direct knockout

Effects of continuum become important at the driplines

arXiv:1412.0491 [nucl-th] (2014)

Spectroscopic factor are strongly correlated to p-h gaps:


## ZNN asymmetry dependence of SF's - Theory

Ab-initio calculations explain the $\mathrm{Z} / \mathrm{N}$ dependence but the effect is much lower than suggested by direct knockout

Effects of continuum become important at the driplines

arXiv:1412.0491 [nucl-th] (2014)

[Hagen et al.
Phys. Rev. Lett. 107, 032501 (2011)]

## Single nucleon transfer in the oxygen chain

[F. Flavigny et al, PRL110, 122503 (2013)]
$\rightarrow$ Analysis of ${ }^{14} \mathrm{O}(d, t)^{13} \mathrm{O}$ 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 asymmetry


## Mapping Ab-Initio calculation into the shell model approach

## Recent works through CCM and IMRSG:

Bogner et al Phys. Rev. Lett. 113, 142501 (2014) Jansen et al Phys. Rev. Lett. 113, 142502 (2014)
$\checkmark$ works well for spectra

## Calculation of observables: need many-body corrections, to evolve operators, add electroweak currents, ect...

See Menendez , Stroberg, Pastore and other talks today...

To have a look at the many-body and effects:

Extract vibration coupling form microscopic calculations...
$C B, T$. Otsuka, in preparation

## "traditional" MBPT approach

PT expansion of effective interactions:


Effective charges (estimate form many-body effects):


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## Some results - ANi chain in pfgor/2 shell

Interaction: NNLO-opt, AV18 (+Gmatrix)
Single particle basis: HF
Preliminar



$B E(2)$ charges


## Some results - ANi chain in pfgg/2 shell

Interaction: NNLO-opt, AV18 (+Gmatrix)
Single particle basis: HF

## Averaged charges


$\rightarrow$ "predicted" charges are smaller than usual phenomenological ones
$\rightarrow$ NO higher
order currents here -- just the many-body correction...

## BE(2) charges

## Some results - $O$ and $C$ chains

## Interaction: N3LO(500) (+Gmatrix)

Single particle basis: HF or HFB
$B E(2)$ charges

|  | C 10 | C 22 | O 14 | O 16 | O 20 |
| :--- | ---: | ---: | ---: | ---: | ---: |
| $\nu_{s 1 / 2}-\nu_{d 3 / 2}:$ | 0.142 | 0.094 | -0.751 | 0.160 | 0.128 |
| $\nu_{s 1 / 2}-\nu_{d 5 / 2}:$ | 0.226 | 0.125 | 0.261 | 0.214 | 0.181 |
| $\nu_{d 3 / 2}-\nu_{d 3 / 2}:$ | 0.278 | 0.121 | 0.198 | 0.082 | 0.155 |
| $\nu_{d 3 / 2}-\nu_{d 5 / 2}:$ | 0.320 | 0.137 | 0.249 | 0.274 | 0.214 |
| $\nu_{d 5 / 2}-\nu_{d 5 / 2}:$ | 0.278 | 0.151 | 0.294 | 0.250 | 0.232 |
| $\pi_{s 1 / 2}-\pi_{d 3 / 2}:$ | 1.131 | 1.051 | 0.594 | 1.105 | 1.078 |
| $\pi_{s 1 / 2}-\pi_{d 5 / 2}:$ | 1.155 | 1.094 | 1.161 | 1.142 | 1.134 |
| $\pi_{d 3 / 2}-\pi_{d 3 / 2}:$ | 1.061 | 1.054 | 1.441 | 0.976 | 1.070 |
| $\pi_{d 3 / 2}-\pi_{d 5 / 2}:$ | 1.141 | 1.107 | 1.042 | 1.091 | 1.170 |
| $\pi_{d 5 / 2}-\pi_{d 5 / 2}:$ | 1.161 | 1.077 | 1.139 | 1.107 | 1.099 |
|  |  |  |  |  |  |
| $\nu_{p 1 / 2}-\nu_{p 3 / 2}:$ | 0.359 | 0.319 | 0.344 | 0.401 | 0.404 |
| $\nu_{p 3 / 2}-\nu_{p 3 / 2}:$ | 0.315 | 0.247 | 0.367 | 0.316 | 0.307 |
|  |  |  |  |  |  |
| $\pi_{p 1 / 2}-\pi_{p 3 / 2}:$ | 1.102 | 1.134 | 1.183 | 1.179 | 1.198 |
| $\pi_{p 3 / 2}-\pi_{p 3 / 2}:$ | 1.128 | 1.103 | 1.075 | 1.056 | 1.082 |

$\rightarrow$ "predicted" charges are smaller than usual phenomenological ones
$\rightarrow$ NO higher order currents here -- just the many-body correction...

## Conclusions

- What to did we learn about realistic chiral forces from ab-initio calculations?
$\rightarrow$ Leading order 3NF are crucial to predict many important features that are observed experimentally (drip lines, saturation, orbit evolution, etc...)
$\rightarrow$ Experimental binding is predicted accurately up to the lower sd shell (A~30) but deteriorates for medium mass isotopes (Ca and above) with roughly 1 MeV/A over binding.
$\rightarrow$ more short-range repulsion or fitting to mid masses will help [see NNLOsat talk, atc...].


## Thank you for your attention!!!!



## Collaborators

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