Near-degenerate systems in nuclear structure and quantum ESNT, 30 March—2 April 2015

## Three-Body Forces and CI Effective Operators in Green's Function Theory

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Formalism and 3NF:
Phys. Rev. C63, 034313 (2001), Phys. Rev. A76, 052503 (2007)
Phys. Rev. C84, 064317 (2011), Phys. Rev. C88, 054326 (2013)
ab-initio \& correlations: Phys. Rev. C89, 061301R (2014)
arXiv:1412.0491 [nucl-th] (2014)

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

24:


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## Current Status of low-energy nuclear physics

Composite system of interacting fermions
Binding and limits of stability
Coexistence of individual and collective behaviors
Self-organization and emerging phenomena EOS of neutron star matter

I) Understanding the nuclear force QCD-derived; 3-nucleon forces (3NFs) First principle (ab-initio) predictions

## III) Interdisciplinary character

Astrophysics
Tests of the standard model Other fermionic systems: ultracold gasses; molecules;

## 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)]
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## Concept of correlations

independent particle picture

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

Particle-vibration so far, fully characterised only isotopes... (!)
stable
[W. Dickhoff, CB, Prog. Part. Null. Phys. 52, 377 (2004)]
[CB and W. H. Dickhoff, Prog. Part. Nucl. Phys 52, 377 (2004)]

## Nuclear forces in exotic nuclei

Nucleon interactions are very complex and difficult to handle

## Change of regime from stable to dripline isotopes !



Symmetric matter:
$\mathrm{N} \approx \mathrm{Z}$
Tensor force (p-n)


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)]

## 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):


## Ab-Initio SCGF approaches

## Coupling single particle to collective modes

- Non perturbative expansion of the self-energy:

- Explicit correlations enter the "three-particle irreducible" propagators:

$$
\begin{aligned}
\Longrightarrow & \equiv \text { particle } \\
& \equiv \text { hole }
\end{aligned}
$$

-Both pp/hh (ladder) and ph (ring) response included -Pauli exchange at 2p1h/2h1p level

## Ionization spectrum of Ne atom

- Both pp and ph configurations are important
- In finite nuclei one need RPA to describe giant resonances
- CANNOT be simply added:


Phys. Rev. A76, 052503 (2007)

## Faddeev RPA method

- Thus, to include both "ladder" and "ring" correlations one must calculate the full $2 \mathrm{p} 1 \mathrm{~h} / 2 \mathrm{~h} 1 \mathrm{p}$ propagator

- In general this is exact if one can calculate the full 6-points Green's function (see lecture of Apr. 13 ${ }^{\text {th }}$ ):



## Faddeev RPA method

- The full $2 p 1 h / 2 h 1 p$ polarization propagator also satisfies a Bethe-Salpeter-like equation:

$$
\begin{aligned}
R_{\alpha \beta \gamma, \mu \nu \lambda}\left(\omega_{1}, \omega_{2}, \omega_{3}\right)= & {\left[g_{\alpha \mu}\left(\omega_{1}\right) g_{\beta \nu}\left(\omega_{2}\right)-g_{\beta \mu}\left(\omega_{2}\right) g_{\alpha \nu}\left(\omega_{1}\right)\right] g_{\lambda \gamma}\left(-\omega_{3}\right) } \\
& +\left(g_{\beta \beta_{1}}\left(\omega_{2}\right) g_{\gamma_{1} \gamma}\left(-\omega_{3}\right) V_{\beta_{1} \sigma, \gamma_{1} \rho} \int \frac{d s}{2 \pi i} R_{\alpha \rho \sigma, \mu \nu \lambda}\left(\omega_{1}, s, \omega_{2}+\omega_{3}-s\right)\right. \\
& +g_{\alpha \alpha_{1}}\left(\omega_{1}\right) g_{\gamma_{1} \gamma}\left(-\omega_{3}\right) V_{\alpha_{1} \sigma, \gamma_{1} \rho} \int \frac{d s}{2 \pi i} R_{\rho \beta \sigma, \mu \nu \lambda}\left(s, \omega_{2}, \omega_{1}+\omega_{3}-s\right) \\
& \left.+\frac{1}{2} g_{\alpha \alpha_{1}}\left(\omega_{1}\right) g_{\beta \beta_{1}}\left(\omega_{2}\right) V_{\alpha_{1} \beta_{1}, \rho \sigma} \int \frac{d s}{-2 \pi i} R_{\rho \sigma \gamma, \mu \nu \lambda}\left(s, \omega_{1}+\omega_{2}-s, \omega_{3}\right)\right)
\end{aligned}
$$

- However, this depends on 4-tmes (3 frequancies) and it is much more complicatde than the p-h Bethe-Salpeter.


## Faddeev RPA method

The full $2 \mathrm{p} 1 \mathrm{~h} / 2 \mathrm{~h} 1 \mathrm{p}$ polarization propagator also satisfies a Bethe-Salpeter-like equation:


Strategy: solve each "pp" and "ph" channel separately, by solving the (simpler) DRPA equations. Then couple to a third line and mix the corresponding amplitudes $\rightarrow$ Faddeev eqs.!!

Faddeev equations for the $2 h 1 p$ motion
Strategy: solve each "pp" and "ph" channel separately, by solving the (simpler) DRPA equations. Then couple to a third line and mix the corresponding amplitudes $\rightarrow$ Faddeev eqs.!!

$$
R^{\text {hap }}(\omega)=\Downarrow \downarrow-\mathbb{A}+R^{1}(\omega)+R^{2}(\omega)+R^{3}(\omega) \quad \begin{aligned}
& \text { Foddeev } \\
& \text { components }
\end{aligned}
$$

Fodder eqns.



## FRPA: Faddeev summation of RPA propagators


-Both pp/hh (ladder) and ph (ring) response included -Pauli exchange at 2p1h/2h1p level

- All order summation through a set of Faddeev equations

where:



## 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



## Accuracy of FRPA - simple atoms/molecules




NB: energies in Hartree errors in mHartree

## Three-nucleon interactions

$\rightarrow$ application to nuclei
$\rightarrow$ need new formalism?
A. Carbone, A. Cipollone, CB, A. Rios, A. PollsPhys. Rev. C88, 054326 (2013).
A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. 111, 062501 (2013).

## 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

pure 3-Body contribution

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


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

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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


- 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)

- 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:


## mons

(a)

(b)

- Third anderPT diagrams with 3BFs:
(a)


(e)

(f)

(g)

(n)




## ADC(n) schemes with 3-body interactions


$\rightarrow$ Adding many-body forces complicates the intermediate states at $3^{\text {rd }}$ order! However, not all terms are equally relevant...
[F. Raimondi, CB, in prep.]

## (Galitskii-Migalal-Boffi-) Koltun sumrule

粦 Koltun sum rule (with NNN interactions):

$$
\sum_{\alpha} \frac{1}{\pi} \int_{-\infty}^{\epsilon_{F}^{-}} d \omega \omega \operatorname{Im} G_{\alpha \alpha}(\omega)=\left\langle\Psi_{0}^{N}\right| \hat{T}\left|\Psi_{0}^{N}\right\rangle+2\left\langle\Psi_{0}^{N}\right| \hat{V}\left|\Psi_{0}^{N}\right\rangle+3\left\langle\Psi_{0}^{N}\right| \hat{W}\left|\Psi_{0}^{N}\right\rangle
$$

粦 Thus, need an extra correction:

$$
E_{0}^{N}=\frac{1}{3 \pi} \int_{-\infty}^{\epsilon_{F}^{-}} \mathrm{d} \omega \sum_{\alpha \beta}\left(2 T_{\alpha \beta}+\omega \delta_{\alpha \beta}\right) \operatorname{Im} G_{\beta \alpha}(\omega)+\frac{1}{3}\left\langle\Psi_{0}^{N}\right| \widehat{V}\left|\Psi_{0}^{N}\right\rangle
$$

or

$$
E_{0}^{N}=\frac{1}{2 \pi} \int_{-\infty}^{\epsilon_{F}^{-}} \mathrm{d} \omega \sum_{\alpha \beta}\left(T_{\alpha \beta}+\omega \delta_{\alpha \beta}\right) \operatorname{Im} G_{\beta \alpha}(\omega)-\frac{1}{2}\left\langle\Psi_{0}^{N}\right| \widehat{W}\left|\Psi_{0}^{N}\right\rangle
$$

$$
\left\langle\Psi_{0}^{N}\right| \widehat{W}\left|\Psi_{0}^{N}\right\rangle \approx \frac{1}{6} \bigcirc
$$

## 3N forces in FRPA/FTDA formalism

$\rightarrow$ Ladder contributions to static self-energy are negligible (in oxygen)


## Equations of Motions with 3NF

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

- EOM for 1-body propagator:

irred. self-energy:
$\rightarrow$

- EOM for 2-body propagator:



## Equations of Motions with 3NF

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

- SC equations for the 4-point GF:


## ladders




## Gorkov and symmetry breaking approaches

V. Somà, CB, T. Duguet, , Phys. Rev. C 89, 024323 (2014)
V. Somà, CB, T. Duguet, Phys. Rev. C 87, 011303R (2013)
V. Somà, T. Duguet, CB, Phys. Rev. C 84, 064317 (2011)
> Ansatz

$$
\ldots \approx E_{0}^{N+2}-E_{0}^{N} \approx E_{0}^{N}-E_{0}^{N-2} \approx \ldots \approx 2 \mu
$$

>Auxiliary many-body state $\left|\Psi_{0}\right\rangle \equiv \sum_{N}^{\text {even }} c_{N}\left|\psi_{0}^{N}\right\rangle$
$\longrightarrow$ Mixes various particle numbers
$\longrightarrow$ Introduce a "grand-canonical" potential $\Omega=H-\mu N$
$\Longrightarrow\left|\Psi_{0}\right\rangle$ minimizes $\Omega_{0}=\left\langle\Psi_{0}\right| \Omega\left|\Psi_{0}\right\rangle$ under the constraint $N=\left\langle\Psi_{0}\right| N\left|\Psi_{0}\right\rangle$
$>$ This approach leads to the following Feynman diagrams:


| 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



## 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:

| ज | 2006 |
| :---: | :---: |
|  | 2010 |
|  | 2012 |
|  | 2013 |
|  | 2014 |

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...)
2015

## Results

## Chiral Hamiltonians for the Oxygen chain



Benchmark with the same initial Hamiltonian

Oxygen dripline including chiral NN +3 N forces correctly reproduced
confirmed in ab-initio calculations by different approaches,
treating explicitly all nucleons as degrees of freedom

Pic. Credit:s
J.Menendez, J.Holt, et al, in prep.

Results from:
Hergert et al. PRL110 242501 (2013),
Cipollone et al. PRL111 062501 (2013), Jansen et al. PRL113 142502 (2014)

## Neutron spectral function of Oxygens



Suncrive

## 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

## 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


## Ca and Ni isotopic chains



$\rightarrow$ Large J in free space SRG matter (must pay attention to its convergence)
$\rightarrow$ Overall conclusions regarding over binding and $\mathrm{S}_{2 n}$ remain but details change

## Two-neutron separation energies for meutron rich $K$ isotopes


$\rightarrow$ Error bar in predictions are from extrapolating the many-body expansion to convergence of the model space.

ISOLTRAP
M. Rosenbusch, et al., PRL (submitted).


## 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...

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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## ${ }^{56} \mathrm{Ni}$ neutron spectral function


W. Dickhoff, CB, Prog. Part. Nucl. Phys. 53, 377 (2004) CB, M.Hjorth-Jensen, Pys. Rev. C79, 064313 (2009)


## 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

|  | C10 | 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 $1 \mathrm{MeV} / \mathrm{A}$ over binding.
$\rightarrow$ more short-range repulsion or fitting to mid masses will help [see NNLOsat, Evgeny talk, and new developments...].
$\rightarrow$ Ab-initio optical potentials are a natutal 'by-product' of the SCGF method.
$\rightarrow$ Earlier investigations of SCGF based optical potentials were very promising; it will now be crucial to apply it in modern ab-initio codes.

Thank you for
your attention!!!

