Near-degenerate systems in nuclear structure and quantum chemistry from ab initio many-body methods ESNT, 30 March—2 April 2015



<u>Three-Body Forces and CI Effective</u> <u>Operators in Green's Function Theory</u>

Carlo Barbieri — University of Surrey

Formalism and 3NF: Phys. Rev. C**63**, 034313 (2001), Phys. Rev. C**84**, 064317 (2011),

Phys. Rev. A**76**, 052503 (2007) 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)









enerale atomicue - enerales atternatives TECHNISCHE UNIVERSITÄT DARMSTADT











A. Cipollone, A. Rios

- V. Somà, T. Duguet
- A. Carbone
- P. Navratil
- A. Polls
- W.H. Dickhoff, S. Waldecker
- D. Van Neck, M. Degroote
- M. Hjorth-Jensen

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

Extreme neutron-proto

Experimental programs RIKEN, FAIR, FRIB

II) Nuclear correlations Fully known for stable isotopes [C. Barbieri and W. H. Dickhoff, Prog. Part. Nucl. Phys **52**, 377 (2004)]

Unst Neutron-rich nuclei; Shell evolution (far from stability)

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

^{brotons}

Be

Li He

neutrons

UNIVERSITY OF

III) Interdisciplinary character *Astrophysics Tests of the standard model Other fermionic systems: ultracold gasses; molecules;*

Extreme mass

Concept of correlations



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

Concept of correlations



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

UNIVERSITY OF

Nuclear forces in exotic nuclei



Example of spectral function ⁵⁶Ni

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

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

...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:



Ionization spectrum of Ne atom



Phys. Rev. A76, 052503 (2007)

UNIVERSITY OF

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



Faddeev RPA method

• Thus, to include both "ladder" and "ring" correlations one must calculate the full 2p1h/2h1p propagator



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



Faddeev RPA method

 The full 2p1h/2h1p polarization propagator also satisfies a Bethe-Salpeter-like equation:

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

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



Faddeev RPA method

The full 2p1h/2h1p 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 2h1p 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.!!



References: CB, et al., Phys. Rev. C63, 034313 (2001); Phys. Rev. A76, 052503 (2007) ERSITY OF

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





UNIVERSITY OF References: CB, et al., Phys. Rev. C63, 034313 (2001); Phys. Rev. A76, 052503 (2007) SURREY

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...

D(2h1p

= hole

(ph)

(ph)

Oll (pp/hh)

R^{(2p1h}

= particle

CB et al., Phys. Rev. C**63**, 034313 (2001) Phys. Rev. A**76**, 052503 (2007) Phys. Rev. C**79**, 064313 (2009)

•A complete expansion requires <u>all</u> <u>types</u> of particle-vibration coupling

"Extended" Hartree Fock

...these modes are all resummed exactly and to all orders in a *ab-initio* many-body expansion.

•The Self-energy $\Sigma^*(\omega)$ yields both single-particle states and scattering

Accuracy of FRPA – simple atoms/molecules

binding, eq. bond distances, \rightarrow ionization energies (molecules)

98-99% of correlation energy is recovered

< 1% of tot. binding energy

		FTDAc	FRPAc	CCSD(T)	FCI	Expt.
H_2						
	E_0	-1.161	-1.161	-1.164	-1.164	-1.175
	r_{H-H}	0.757	0.757	0.761		0.741
	I	16.03	16.03	16.12		16.08
BeH_2						
	E_0	-15.831	-15.832	-15.835	-15.836	-
	r_{Be-H}	1.337	1.337	1.339		1.340
	I	11.78	11.76	11.89		-
HCl						
	E_0	-460.256	-460.255	-460.254		-
	r_{H-Cl}	1.297	1.293	1.290		1.275
	I	12.24	12.24	12.26		-
$_{\mathrm{HF}}$						
	E_0	-100.224	-100.228	-100.228	-100.231	-
	r_{H-F}	0.916	0.913	0.920		0.917
	I	15.70	15.54	15.42		16.12
H_2O						
	E_0	-76.240	-76.236	-76.241		-
	r_{H-O}	0.964	0.962	0.967		0.958
	Λ_{O-H-O}	102	102	102		104
	I	12.15	12.21	11.94		12.61
					-	

binding energies (atoms)

	Hartree-Fock	FTDA	FRPA	CCSD	Experiment
Не	-2.8617(+42.0)	-2.9028(+0.9)	-2.9029(+0.8)	-2.9039(-0.2)	-2.9037
Be ²⁺	-13.6117(+43.9)	-13.6559(-0.3)	-13.6559(-0.3)	-13.6561(-0.5)	-13.6556
Be	-14.5731(+94.3)	-14.6438(+23.6)	-14.6436(+23.8)	-14.6522(+15.2)	-14.6674
Ne	-128.5505(+387.8)	-128.9343(+4.0)	-128.9381(+0.2)	-128.9353(+3.0)	-128.9383
Mg ²⁺	-198.837(+444)	-199.226(-5)	-199.228(-7)	-199.225(-4)	-199.221
Mg	-199.616(+438)	-200.048(+6)	-200.052(+2)	-200.050(+4)	-200.054
Ar	-526.820(+724)	-527.543(+1)	-527.548(-4)	-527.536(+8)	-527.544
$\sigma_{\rm rms}$ [mH]	392	9.5(3.6)	9.5(3.4)	6.9(4.2)	

NB: energies in Hartree errors in mHartree

Degroote, Ofvan Neck, C. B. Phys. Rev. A 83, 042517 (2011); 85, 012501 (2012)]

Three-nucleon interactions

→ application to nuclei
→ 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).





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

* NNN forces can enter diagrams in three different ways:



Correction to external 1-Body interaction



Correction to <u>non-contracted</u> 2-Body interaction



pure 3-Body contribution

- Contractions are with <u>fully correlated density</u> <u>matrices</u> (BEYOND a normal ordering...)





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

* NNN forces can enter diagrams in three different ways:





Inclusion of NNN forces

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

* NNN forces can enter diagrams in three different ways:

→ Define new 1- and 2-body interactions and use <u>only</u> interaction-irreducible diagrams



 Contractions are with <u>fully correlated density matrices</u> (BEYOND a normal ordering...)



Inclusion of NNN forces

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

- Second order PT diagrams with 3BFs:

(b)

effectively.



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:





- Third order PT diagrams with 3BFs: (0)(n)

FIG. 5. 1PI, skeleton and interaction irreducible self-energy diagrams appearing at 3^{rd} -order in perturbative expansion (7), making use of the effective hamiltonian of Eq. (9).



ADC(n) schemes with 3-body interactions



→ Adding many-body forces complicates the intermediate states at 3rd order! However, not all terms are equally relevant...

[F. Raimondi, CB, in prep.]



% Koltun sum rule (with NNN interactions):

* Thus, need an extra correction:

$$E_0^N = \frac{1}{3\pi} \int_{-\infty}^{\epsilon_F^-} \mathrm{d}\omega \, \sum_{\alpha\beta} (2T_{\alpha\beta} + \omega\delta_{\alpha\beta}) \mathrm{Im} \, G_{\beta\alpha}(\omega) + \frac{1}{3} \langle \Psi_0^N | \hat{V} | \Psi_0^N \rangle$$

or

$$E_0^N = \frac{1}{2\pi} \int_{-\infty}^{\epsilon_F} \mathrm{d}\omega \, \sum_{\alpha\beta} (T_{\alpha\beta} + \omega\delta_{\alpha\beta}) \mathrm{Im} \, G_{\beta\alpha}(\omega) - \frac{1}{2} \langle \Psi_0^N | \widehat{W} | \Psi_0^N \rangle$$





3N forces in FRPA/FTDA formalism

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



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



Equations of Motions with 3NF

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



irred. self-energy:



- EOM for 2-body propagator:





Equations of Motions with 3NF

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





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
$$(... \approx E_0^{N+2} - E_0^N \approx E_0^N - E_0^{N-2} \approx ... \approx 2\mu)$$

> Auxiliary many-body state $|\Psi_0
angle \equiv \sum_N^{\mathrm{even}} c_N |\psi_0^N
angle$

Mixes various particle numbers

ightarrow Introduce a "grand-canonical" potential $\ \ \Omega = H \! - \! \mu N$

 $\implies |\Psi_0\rangle$ minimizes $\Omega_0 = \langle \Psi_0 | \Omega | \Psi_0 \rangle$ under the constraint $N = \langle \Psi_0 | N | \Psi_0 \rangle$

This approach leads to the following Feynman diagrams:





Truncation scheme:	Dyson formulation (closed shells)	Gorkov formulation (semi-magic)
1 st order:	Hartree-Fock	HF-Bogolioubov
2 nd order:	2 nd order	2 nd order (w/ pairing)
 3 rd and all-orders sums, P-V coupling:	ADC(3) FRPA etc	G-ADC(3) work in progress







Ab-initio Nuclear Computation & BcDor code







Chiral Hamiltonians for the Oxygen chain



Pic. Credit:s

UNIVERSITY OF

J.Menendez, J.Holt, et al, in prep.

Benchmark with the same initial Hamiltonian

Oxygen dripline including chiral NN +3N forces correctly reproduced

confirmed in ab-initio calculations by different approaches,

treating explicitly all nucleons as degrees of freedom

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



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)



> cf. microscopic shell model [O[·] et al, PRL**105**, 032501 (2010).]



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

→ cf. microscopic shell model [Otsuka et al, PRL105, 032501 (2010).]

UNIVERSITY OF $\frac{N3LO (\Lambda = 500 \text{Mev/c}) \text{ chiral NN interaction evolved to 2N + 3N forces (2.0 \text{fm}^{-1})}{N2LO (\Lambda = 400 \text{Mev/c}) \text{ chiral 3N interaction evolved (2.0 \text{fm}^{-1})}$

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 ¹⁴O(d,t)¹³O and ¹⁴O(d,³He)¹³N transfer reactions @ SPIRAL

Reaction	<i>E</i> * (MeV)	J^{π}	R ^{HFB} (fm)	<i>r</i> ₀ (fm)	$C^2 S_{exp}$ (WS)	$\frac{C^2 S_{\rm th}}{0p + 2\hbar\omega}$	R _s (WS)	$C^2 S_{exp}$ (SCGF)	$C^2 S_{\rm th}$ (SCGF)	R _s (SCGF)
$^{14}O(d, t)$ ^{13}O	0.00	3/2-	2.69	1.40	1.69 (17)(20)	3.15	0.54(5)(6)	1.89(19)(22)	3.17	0.60(6)(7)
14 O (<i>d</i> , 3 He) 13 N	0.00	$1/2^{-}$	3.03	1.23	1.14(16)(15)	1.55	0.73(10)(10)	1.58(22)(2)	1.58	1.00(14)(1)
	3.50	$3/2^{-}$	2.77	1.12	0.94(19)(7)	1.90	0.49(10)(4)	1.00(20)(1)	1.90	0.53(10)(1)
16 O (<i>d</i> , <i>t</i>) 15 O	0.00	$1/2^{-}$	2.91	1.46	0.91(9)(8)	1.54	0.59(6)(5)	0.96(10)(7)	1.73	0.55(6)(4)
16 O (<i>d</i> , 3 He) 15 N [19,20]	0.00	$1/2^{-}$	2.95	1.46	0.93(9)(9)	1.54	0.60(6)(6)	1.25(12)(5)	1.74	0.72(7)(3)
	6.32	$3/2^{-}$	2.80	1.31	1.83(18)(24)	3.07	0.60(6)(8)	2.24(22)(10)	3.45	0.65(6)(3)
18 O (<i>d</i> , 3 He) 17 N [21]	0.00	$1/2^{-}$	2.91	1.46	0.92(9)(12)	1.58	0.58(6)(10)			





- Overlap functions and strengths from GF

- Rs independent of asymmetry

Ca and Ni isotopic chains



→ Large J in free space SRG matter (must pay attention to its convergence) → Overall conclusions regarding over binding and S_{2n} remain but details change



Two-neutron separation energies for neutron rich K isotopes



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)

✓ works well for spectra

Calculation of observables: <u>need many-body corrections, to evolve operators,</u> <u>add electroweak currents, ect...</u>

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

Extract vibration coupling form microscopic calculations...



"traditional" MBPT approach

PT expansion of effective interactions:



Effective charges (estimate form many-body effects):





⁵⁶Ni neutron spectral function



W. Dickhoff, CB, Prog. Part. Nucl. Phys. 53, 377 (2004) CB, M.Hjorth-Jensen, Pys. Rev. C**79**, 064313 (2009)





Dressed (self consistent) propagator:



PT expansion of effective interactions:



but NO self-en insertions

Effective charges (many-body contributions):

JNIVERSITY OF



Some results - ^ANi chain in pfg_{9/2} shell

Interaction: NNLO-opt, AV18 (+Gmatrix)

Single particle basis: HF



Some results - ^ANi chain in pfg_{9/2} shell

Interaction: NNLO-opt, AV18 (+Gmatrix)

Single particle basis: HF

Averaged charges



Preliminary

→ "predicted" charges are smaller than usual phenomenological ones

→ NO higher order currents here -- just the many-body correction...

Some results - O and C chains

Interaction: N3LO(500) (+Gmatrix)

Single particle basis: HF or HFB

	C10	C22	014	O16	O20
$ u_{s1/2} $ - $ u_{d3/2}$:	0.142	0.094	-0.751	0.160	0.128
$ u_{s1/2} $ - $ u_{d5/2}$:	0.226	0.125	0.261	0.214	0.181
$\nu_{d3/2}$ - $\nu_{d3/2}$:	0.278	0.121	0.198	0.082	0.155
$\nu_{d3/2}$ - $\nu_{d5/2}$:	0.320	0.137	0.249	0.274	0.214
$ u_{d5/2} $ - $ u_{d5/2}$:	0.278	0.151	0.294	0.250	0.232
$\pi_{s1/2}$ - $\pi_{d3/2}$:	1.131	1.051	0.594	1.105	1.078
$\pi_{s1/2}$ - $\pi_{d5/2}$:	1.155	1.094	1.161	1.142	1.134
$\pi_{d3/2}$ - $\pi_{d3/2}$:	1.061	1.054	1.441	0.976	1.070
$\pi_{d3/2}$ - $\pi_{d5/2}$:	1.141	1.107	1.042	1.091	1.170
$\pi_{d5/2}$ - $\pi_{d5/2}$:	1.161	1.077	1.139	1.107	1.099
$ u_{p1/2} $ - $ u_{p3/2}$:	0.359	0.319	0.344	0.401	0.404
$ u_{p3/2} $ - $ u_{p3/2}$:	0.315	0.247	0.367	0.316	0.307
$\pi_{p1/2}$ - $\pi_{p3/2}$:	1.102	1.134	1.183	1.179	1.198
$\pi_{p3/2}$ - $\pi_{p3/2}$:	1.128	1.103	1.075	1.056	1.082

E(2) charges

→ "predicted" charges are smaller than usual phenomenological ones

→ NO higher order currents here -- just the many-body correction...



Conclusions

IVERSITY OF

•What to did we learn about realistic chiral forces from ab-initio calculations?

- → Leading order 3NF are crucial to predict many important features that are observed experimentally (drip lines, saturation, orbit evolution, etc...)
- → 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.

50

30

32

30

26 28

24

N

20

[MeV]

Thank ya

- → more short-range repulsion or fitting to mid masses will help [see NNLOsat, Evgeny talk, and new developments...].
- → Ab-initio optical potentials are a natutal 'by-product' of the SCGF method.
- → Earlier investigations of SCGF based optical potentials <u>were very</u> <u>promising</u>; it will now be crucial to apply it in modern ab-initio codes.