

Recent Advances in SCGF Calculations

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2 March 2017





- Some details of the current SCGF formalism (extensions for 3NFs)
- Application of saturating interactions and new local-nonlocal force
- Bubble structure of ³⁴Si
- occupation of valence shells
- Nuclei from Lattice QCD (at $m_{\pi}=0.47 \text{ GeV/}c^2 \dots$)

Related calculations (see following talks):

- Shell model effective charges
- Dipole response
- Ab-Initio optical potential from SCGF



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 Experimental programs RIKEN, FAIR, FRIB

Unstable nuclei

~3,200 known isotopes

Extreme mass

r-process path...

- ~7,000 predicted to exist
- Correlation characterised in full for ~283 stable

Nature 473, 25 (2011); 486, 509 (2012)



Be Li He

neutrons

brotons

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

Self-Consistent Green's Function Approach



• Global picture of nuclear dynamics

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- Reciprocal correlations among effective modes
- Guaranties macroscopic conservation laws

Self-Consistent Green's Function Approach



Gorkov and 3-nucleon forces





Truncation scheme:	Dyson formulation (closed shells)	Gorkov formulation (semi-/doubly-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
This is a <u>non-perturba</u> <u>all-orders resummation</u> — NOT a PT truncation	n <u>tive</u> on n!	
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Inclusion of NNN forces

- Second order PT diagrams with 3BFs:



- Use of irreducible 2-body interactions
- Need to correct the Koltun sum rule (for energy)

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 3p2h/3h2p terms relevant to next-generation high-precision methods.

A. Carbone, CB, et al., Phys. Rev. C88, 054326 (2013) and F. Raimondi, CB, in preparation (2017).

- Third order PT diagrams with 3BFs:



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).



- Second order PT diagrams with 3BFs: A. Carbone, CB, et al., Phys. Rev. C88, 054326 (2013) and F. Raimondi, CB, in preparation (2017).

- Third order PT diagrams with 3BFs:







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Inclusion of NNN forces

First interactions irreducible 3NF term:



F. Raimondi, CB, arXiv:1701.08127v1 [nucl-th] and PhysRevC in preparation (2017). Including 3N forces in the many-body diagrammatic with the ADC formalism 13

while the one connecting through a hole-particle (hp) interaction gives

$$\begin{split} \mathbf{D}^{hp}_{(k_{1}k_{2}n_{3}),(k_{4}k_{5}n_{6})} &= \frac{1}{2} \left((\mathcal{Y}^{k}_{\mu}\mathcal{X}^{n}_{\rho})^{*} \widetilde{V}_{\mu\nu,\lambda\rho} \mathcal{Y}^{k}_{\lambda}\mathcal{X}^{n}_{\nu} \delta_{k_{1}k_{4}} \right. \\ &- (\mathcal{Y}^{k}_{\mu}\mathcal{X}^{n}_{\rho})^{*} \widetilde{V}_{\mu\nu,\lambda\rho} \mathcal{Y}^{k}_{\lambda}\mathcal{X}^{n}_{\nu} \delta_{k_{1}k_{5}} \\ &- (\mathcal{Y}^{k}_{\mu}\mathcal{X}^{n}_{\rho})^{*} \widetilde{V}_{\mu\nu,\lambda\rho} \mathcal{Y}^{k}_{\lambda}\mathcal{X}^{n}_{\nu} \delta_{k_{2}k_{4}} \\ &+ (\mathcal{Y}^{k}_{\mu}\mathcal{X}^{n}_{\rho})^{*} \widetilde{V}_{\mu\nu,\lambda\rho} \mathcal{Y}^{k}_{\lambda}\mathcal{X}^{n}_{\nu} \delta_{k_{2}k_{5}} \end{split}$$

We now turn to the Feynman diagram of Fig. 3c, which is the focus work. To our knowledge the ADC formulas arising from this term presented before. The Feynman rules give the following expression for

$$\Sigma^{(3c)}_{\alpha\beta}(\omega) = -\frac{(\hbar)^4}{4} \int \frac{d\omega_1}{2\pi i} \int \frac{d\omega_2}{2\pi i} \int \frac{d\omega_3}{2\pi i} \int \frac{d\omega_4}{2\pi i} \sum_{\substack{\gamma \delta \nu \mu \epsilon \lambda \\ \epsilon \rho \sigma \sigma \gamma}} \widetilde{V}_{\alpha\gamma, \delta\nu} g_{\xi\gamma}(\omega_3) g_{\gamma}(\omega_3)$$

 $g_{\delta\epsilon}(\omega_1) W_{\mu\epsilon\lambda,\xi\eta\theta} g_{\theta\tau}(\omega - \omega_2 + \omega_4) g_{\eta\sigma}(\omega_2) g_{\chi\mu}(\omega_4) \widetilde{V}_{\sigma\tau}$

By performing the four integrals in the complex plane, we find six term ing to the different time orderings of the three interactions. Altogether

$$\begin{split} \Sigma^{(3c)}_{\alpha\beta}(\omega) &= \frac{1}{4} \sum_{\substack{\gamma\delta,\nu\mu\kappa\lambda\\\xi\eta\sigma,\chi}} \widetilde{V}_{\alpha\gamma,\delta\nu} W_{\epsilon\lambda\mu,\eta\theta\xi} \widetilde{V}_{\sigma\tau,\delta\chi} \times \\ &\left(-\sum_{\substack{n_1n_2k_3\\n_4n_5k_6}} \frac{(\lambda_{\delta}^{n_1} \lambda_{\nu}^{n_2} \mathcal{Y}_{\gamma}^{n_3})^* \lambda_{\epsilon}^{n_1} \lambda_{\lambda}^{n_2} \mathcal{Y}_{\xi}^{k_3} (\lambda_{\eta}^{n_4} \lambda_{\theta}^{n_5} \mathcal{Y}_{\mu}^{n_3})^* \lambda_{\tau}^{n_4} \lambda_{\tau}^{n_7} \\ &+ \sum_{\substack{n_1n_2k_3\\n_4n_5k_6}} \frac{\mathcal{Y}_{\delta}^{h_2} \mathcal{Y}_{\nu}^{n_3} (\mathcal{Y}_{\epsilon}^{h_2} \mathcal{Y}_{\lambda}^{n_2} \mathcal{Y}_{\lambda}^{h_2} \mathcal{Y}_{\lambda}$$

where the first (last) three terms correspond to forward-in-time (bac Goldstone diagrams.



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Figure 5: Diagrams of the ADC(3) coupling matrices with one effective 2NF \tilde{V} and one interaction-irreducible 3NF \tilde{W} . The coupling matrix (a) is linked to 2plh ISCs and corresponds to Eq. (45), while (b) is linked to 2h1p ISCs and corresponds to Eq. (46).

By comparing to the third order terms in Eq. (24), one see that the new contributions to the coupling matrices contain one effective 2NF and one interactionirreducible 3NF. The following forward-in-time matrix can be singled out from either the second or third line of Eq. (44),

$$\mathbf{M}_{(n_1n_2k_3)\alpha}^{(2N 3N a)} \equiv \frac{1}{2\sqrt{2}} \frac{X_{\xi}^{e_1} \mathcal{X}_{\rho_1}^{e_1} \mathcal{X}_{\sigma_2}^{e_2} W_{\xi\rho\sigma,\zeta\eta\theta} \mathcal{Y}_{\xi}^{e_3} \mathcal{Y}_{\eta}^{e_3} \mathcal{Y}_{\theta}^{e_6}}{\varepsilon_{\pi_1}^{e_1} - \varepsilon_{\pi_2}^{+} - \varepsilon_{\pi_3}^{+}} \left(\mathcal{Y}_{\mu\nu}^{k_2} \mathcal{Y}_{\nu}^{k_2} \mathcal{X}_{\lambda}^{n_4} \right)^* \tilde{V}_{\mu\nu,\alpha\lambda} , \quad (45)$$

while in the last two lines of Eq. (44) we read the backward-in-time coupling matrix:

$$\mathbf{N}_{\alpha(k_1k_2n_3)}^{(2N \ 3N \ a)} \equiv -\frac{1}{2\sqrt{2}} \widetilde{V}_{\alpha\lambda,\mu\nu} \left(\mathcal{Y}_{\lambda}^{k_4} \mathcal{X}_{\mu}^{n_5} \mathcal{X}_{\nu}^{n_6} \right)^* \frac{\mathcal{X}_{\sigma}^{n_3} \mathcal{X}_{\sigma}^{n_5} \mathcal{X}_{\varepsilon}^{n_6}}{\varepsilon_{k_1}^- + \varepsilon_{k_2}^- - \varepsilon_{n_3}^+ - \varepsilon_{n_5}^+ - \varepsilon_{n_6}^+}. \quad (46)$$

The diagrammatic representations of Eqs. (45) and (46) are displayed in Fig. 5. The only interaction matrix that connects 2p1h ISCs through a 3NF is found from the first term of Eq. (44).

$$\mathcal{C}^{3N}_{(n_1 n_2 k_3),(n_4 n_5 k_6)} \equiv -\frac{1}{2} \mathcal{X}^{n_1}_{\nu} \mathcal{X}^{n_2}_{\mu} \mathcal{Y}^{k_3}_{\rho} W_{\nu\mu\lambda,\epsilon\eta\rho} \left(\mathcal{X}^{n_4}_{\epsilon} \mathcal{X}^{n_5}_{\eta} \mathcal{Y}^{k_6}_{\lambda} \right)^* , \qquad (47)$$

which is explicitly antisymmetric in the particle indexes. With Eqs. (47) and (27) we can rewrite the first term of Eq. (44) as,

$$\mathbf{M}_{\alpha r}^{\dagger (I-2N)} \frac{1}{\hbar \omega - E_r} \mathbf{C}_{rr'}^{3N} \frac{1}{\hbar \omega - E_{r'}} \mathbf{M}_{r'\beta}^{(I-2N)} .$$
(48)

The expression (48) contains only the first order contribution in the interaction matrix expansion, corresponding to the second term in the r.h.s. of Eq. (23), for $B = \mathbf{C}^{3N}$. This is resummed to all order by diagonalizing the Dyson matrix (19), which will automatically include *all* the higher order terms in the expansion.

From the fourth term of Eq. (44), we single out the only backward-in-time interaction matrix connecting two 2h1p configurations through a 3N interaction, that is

$$\mathbf{D}_{(k_1k_2n_3),(k_4k_5n_6)}^{3N} \equiv -\frac{1}{2} \left(\mathcal{Y}_{\nu}^{k_1} \mathcal{Y}_{\mu}^{k_2} \mathcal{X}_{\rho}^{n_3} \right)^* W_{\nu\mu\lambda,\epsilon\eta\rho} \, \mathcal{Y}_{\epsilon}^{k_4} \mathcal{Y}_{\eta}^{k_5} \mathcal{X}_{\lambda}^{n_6} \,, \tag{49}$$

which is also explicitly antisymmetric in the hole indexes. With Eqs. (49) and (28) we associate the fourth term of Eq. (44) to

$$\mathbf{N}_{\alpha s}^{(I-2N)} \frac{1}{\hbar \omega - E_s} \mathbf{D}_{ss'}^{3N} \frac{1}{\hbar \omega - E_{s'}} \mathbf{N}_{s'\beta}^{\dagger (I-2N)}$$
. (50)



Ab-initio Nuclear Computation & BcDor code



Ab-initio Nuclear Computation & BcDor code

http://personal.ph.surrey.ac.uk/~cb0023/bcdor/

Computational Many-Body Physics





Download

Documentation

Welcome

From here you can download a public version of my self-consistent Green's function (SCGF) code for nuclear physics. This is a code in J-coupled scheme that allows the calculation of the single particle propagators (a.k.a. one-body Green's functions) and other many-body properties of spherical nuclei. This version allows to:

- Perform Hartree-Fock calculations.
- Calculate the the correlation energy at second order in perturbation theory (MBPT2).
- Solve the Dyson equation for propagators (self consistently) up to second order in the self-energy.
- Solve coupled cluster CCD (doubles only!) equations.

When using this code you are kindly invited to follow the creative commons license agreement, as detailed at the weblinks below. In particular, we kindly ask you to refer to the publications that led the development of this software.

Relevant references (which can also help in using this code) are: Prog. Part. Nucl. Phys. 52, p. 377 (2004), Phys. Rev. A76, 052503 (2007), Phys. Rev. C79, 064313 (2009), Phys. Rev. C89 024323 (2014)



Results for the N-O-F chains

A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013) and Phys. Rev. C **92**, 014306 (2015)



 \rightarrow 3NF crucial for reproducing binding energies and driplines around oxygen

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

UNIVERSITY OF N3LO (Λ = 500Mev/c) chiral NN interaction evolved to 2N + 3N forces (2.0fm⁻¹) N2LO (Λ = 400Mev/c) chiral 3N interaction evolved (2.0fm⁻¹)



V. Somà, CB et al. Phys. Rev. C89, 061301R (2014)

Two-neutron separation energies predicted by chiral NN[EM(500)]+3NF[N2LO(400)]:



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→ First ab-initio calculation over a contiguous portion of the nuclear chart—open shells are now possible through the Gorkov-GF formalism

proton radii

matter radii

Ş

Radii and Binding Energies in Oxygen Isotopes: A Challenge for Nuclear Forces

V. Lapoux,^{1,*} V. Somà,¹ C. Barbieri,² H. Hergert,³ J. D. Holt,⁴ and S. R. Stroberg⁴



2.4

2.2

14

16

18

AO

20

22

24

FIG. 1. Oxygen binding energies. Results from SCGF and IMSRG calculations performed with EM [20–22] and NNLO_{sat} [26] interactions are displayed along with available experimental data.





Size of radii not prefect but remains overall correct throughout the *pf* shell with NNLO-sat.

This suggests that saturation is indeed under control.

→ Improvements of many-body truncations beyond 2nd order Gorkov will also be relevant. (work in progress!)



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Bubble nuclei... ³⁴Si prediction



Duguet, Somà, CB, et al. arXiv:1611.08570 [nucl-th]

- ³⁴Si is unstable, charge distribution still unknown
- Suggested central depletion from mean-field simulations
- Ab-initio theory confirms predictions

<u>Validated</u> by charge distributions and neutron quasiparticle spectra:







A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013) and Phys. Rev. C **92**, 014306 (2015) and *in preparation*

More in detail:

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Quenching of absolute spectroscopic factors



Z/N asymmetry dependence of SFs - Theory

Ab-initio calculations explain (a very weak) the Z/N dependence but the effect is much lower than suggested by direct knockout

Rather the quenching is high correlated to the gap at the Femi surface.



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A. Cipollone, CB, P Navrátil Phys. Rev. C**92**, 014306 (2015)

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CB, M. Hjorth-Jensen, Phys. Rev. C **79**, 064313 (2009) Local vs. non-local chiral N²LO NNN interaction — by P. Navrátil

• Local: chiral N³LO NN+ N²LO 3N500

 $\begin{array}{c} & & \\ \hline \\ \pi \\ \hline \\ c_1, c_3, c_4 \end{array} \qquad \begin{array}{c} & \\ \hline \\ c_D \end{array} \qquad \begin{array}{c} \\ \hline \\ c_E \end{array}$

<H>=-28.4939 <V3b_2pi>= -5.8819 <V3b_D>= -0.2206 <V3b_E>= 1.2665

- Non-local: chiral N²LO_{sat} NN+3N
 - c_{D} =+0.8168 c_E=-0.0396 (³H E_{gs}=-8.53 MeV)
 - ⁴He

<H>=-28.4596 <V3b_2pi>= -4.7260 <V3b_D>= 1.3897 <V3b_E>= 0.4174

• Local/Non-local: chiral N³LO NN+ N²LO

 $F(\frac{1}{2}(\pi_1^2 + \pi_2^2); \Lambda_{\text{nonloc}}) W_1^Q(\Lambda_{\text{loc}}) F(\frac{1}{2}(\pi_1^2 + \pi_2^2); \Lambda_{\text{nonloc}}) \leq$

Use completeness in HO basis to calculate products of *F W F*

-
$$c_D = +0.7$$
 $c_E = -0.06$ (³H $E_{gs} = -8.44$ MeV)

– ⁴He

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<H>=-28.2530 <V3b_2pi>= -4.8124 <V3b_D>= 0.7414 <V3b_E>= 0.4255

N3LO(500) + nln 3NF

SCGF – Gorkov-ADC(2)



<u>PRELIMINARY</u>



Study of nuclear interactions from Lattice QCD

In collaboration with:





Approaches to nuclei from LQCD $L = -\frac{1}{\varDelta} G^a_{\mu\nu} G^{\mu\nu}_a + \bar{q} \gamma^{\mu} (i \partial_{\mu} - g t^a A^a_{\mu}) q - m \bar{q} q$ gluons $U = e^{iaA_{\mu}}$ quarks q on the sites on the links Yukawa (1930s) 4-dim **Euclid** Lattice а Fujita-Miyazawa (1950s) UNIVERSITY OF **Nucleus**

Why nuclear interactions on the Lattice??

- Extend LQCD beyond few-bodies
- Not based on a specific EFT momentum scale

 exploitable to high densities (e.g. Neutron stars)
- No LECs to worry about ...but:
- Variation in potentials from variation in sink operators (→ estimation of theoretical uncertainties)
- Direct derivation of hyperon-nucleon interactions
- 3NF can be derived consistently with NN interactions

Need to develop appropriate many-body methods





Two-Nucleon HAL potentials



Quark mass dependence of V(r) for NN partial wave $({}^{1}S_{0}, {}^{3}S_{1}, {}^{3}S_{1} - {}^{3}D_{1})$

→ Potentials become stronger m_{π} as decreases.



(Finite-T results by A. Carbone, priv. comm.)

Analysis of Brueckner HF

Scattering of two nucleons outside the Fermi sea (\rightarrow BHF):



Mixed SCGF-Brueckner approach

Solve full many-body dynamics in model space (P+Q') and the Goldstone's ladders outside it (i.e. in Q'' only):



Treating short-range corr. with a G-matrix

 The short-range core can be treated by summing ladders outside the model space:

Two contributions to the derivative:

- $\Sigma_{\alpha\beta}^{MF}(\omega)$ is due to scattering to (high-k) states in the Q space
- $\Sigma(\mathbf{r},\mathbf{r}';\omega)$ accounts for low-energy (long range) correlations
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(Galitskii-Migdal-Boffi-) Koltun sumrule

* Koltun sum rule (with NNN interactions):



Benchmark on ⁴He

C. McIlroy, CB, et al., arXiv:1701.02607 [nucl-th]



Can benchmark the Gmtx+ADC(3) method on light ⁴He, where exact solutions are possible:

	G(ω) + ADC(3)	Exact
HALQCD @ m _π ≈470MeV	4.79(3) MeV	5.09 MeV ¹
1		

¹H. Nemura et al., Int. J. Mod. Phys. E 23, 1461006 (2014)

→ Can expect accuracy on binding energies at about 10%

$$G'(\omega) = V + \int dk_a dk_b V \frac{\hat{Q}''}{\omega - \varepsilon(k_a) - \varepsilon(k_b) + i\eta} G''(\omega)$$
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SUBREY

Binding of ¹⁶O and ⁴⁰Ca:

C. Mcllroy, CB, et al., arXiv:1701.02607 [nucl-th]



Binding energies are ~17 MeV ¹⁶O and 70-75MeV for ⁴⁰Ca. Possibly being underestimated by 10%

→	¹⁶ O at m _π ≈ 470	MeV is	unstable toward	4-α	breakup!
_	π				

	E_0^A [MeV]	⁴ He	¹⁶ O	⁴⁰ Ca
	BHF [22]	-8.1	-34.7	-112.7
	$G(\omega) + ADC(3)$	-4.80(0.03)	-17.9 (0.3) (1.8)	-75.4 (6.7) (7.5)
[C.S.McIlrov C.B. HAL coll in prep]	Exact Result [51]	-5.09	_	_
	Separation into ⁴ He clusters:		-2.46 (0.3) (1.8)	24.5 (6.7) (7.5)
				-75.4 (6.7) (7.5) - 24.5 (6.7) (7.5)

Infrared convergence







Results for binding



C. Mcllroy, CB, et al., arXiv:1701.02607 [nucl-th]

Matter distribution of ¹⁶O and ⁴⁰Ca:



Calculated matter radii at $m_{\pi} \approx 470$ MeV:

		¹⁶ O	⁴⁰ Ca
r _{pt-matter} :	BHF [22]	2.35 fm	2.78 fm
F ·	HF	2.39 fm	2.78 fm
	$G(\omega) + ADC(3)$	2.64 fm	2.97 fm
r _{charge} :	$G(\omega) + ADC(3)$	2.77 fm	3.08 fm
-	Experiment [54, 55]	2.73 fm	3.48 fm



C. Mcllroy, CB, et al., arXiv:1701.02607 [nucl-th]

Spectral strength in ¹⁶O and ⁴⁰Ca:



C. McIlroy, CB, et al., arXiv:1701.02607 [nucl-th]

Spectral strength in ¹⁶O and ⁴⁰Ca:



C. McIlroy, CB, et al., arXiv:1701.02607 [nucl-th]

Future application for Ys in nuclei now possible

- Physical mass now under reach ($m_{\pi} \approx 145 \text{ MeV}$) for hyperons
- Need to improve on statistic for the NN sector
- $\Omega\Omega$ potential $NN(^{3}S_{1})$ tensor potential 100 200 t=16 **Potential** OPEP[lat] AV18[phen] t=17 t=08 t=18 t = 0.950 t=10 100 V(r) [MeV] V(r) [MeV] 0 0 -100 -50 relimin -200 0.5 -100 1.5 2 2.5 n 1 3 0.5 2.5 0 1.5 3 1 r [fm] r [fm]

HALQCD coll. -- Talk of S. Aoki at Kavli institute, Oct. 2016



Summary

Mid-masses and chiral interactions:

- → 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.
- → New fits of chiral interaction are promising for low-energy observables and for scattering (see A. Idini, next).

HALQCD Nuclear forces:

→ Strong short range behavior calls for new ideas in ab-initio many-body methods. Diagram resummation through G-matrix is good starting point (to be extended)



→ At m_{π} =469MeV, closed shell 4He, 16O and 40Ca are bound. But oxygen is unstable toward 4- α break up, calcium stays bound. Underestimation of radii increases with A do to large saturation density (as for EM(500)+NLO3NF).

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- *A. Cipollone, C. Mcllroy A. Rios, A. Idini, F. Raimondi*
- V. Somà, T. Duguet



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atomique + energies alternati







S. Aoki, **T. Doi, T. Hatsuda**, Y. Ikeda, **T. Inoue**, N. Ishii, K. Murano, **H. Nemura**, K. Sasaki F. Etminan T. Miyamoto, T. Iritani S. Gongyo





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