Computational Advances in Nuclear and Hadron Physics (CANHP 2015) @

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Green's function studies of medium-mass nuclei and Lattice QCD interactions

Carlo Barbieri — University of Surrey

Part I – Applications of the SCGF approach:

- Structure of oxygen's chain isotopes
- notes on spectroscopic factors
- Neutron rich Calciums and neighbors



Phys. Rev. C 92, 014306 (2015)

Part II – Applications of the SCGF approach:

Results for nuclear forces from LCQD
 SCGF approach to handle short-range repulsion.





- **A. Cipollone**, A. Rios, F. Raimondi
- V. Son





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ie atomique + energies alternativ







- 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
- YITP Kyoto Univ. RIKEN Nishina Nihon Univ. RCNP Osaka Univ Univ. Tsukuba Univ. Birjand Univ. Tsukuba Stony Brook Univ. YITP Kyoto Univ.



University in St.Louis

Center for Molecular Modeling

M. Hjorth-Jensen

W.H. Dickhoff, S. Waldecker

A. Polls

D. Van Neck, **M. Degroote**



Spectroscopy via knock out reactions-basic idea

Use a probe (ANY probe) to eject the particle we are interested to:



Concept of correlations



Understood for a few stable closed shells: [CBugedow H. Dickhoff, Prog. Part. Nucl. Phys **52**, 377 (2004)] SURREY

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Concept of correlations



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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

Extreme neutron-protos

Experimental programs RIKEN, FAIR, FRIB

Extreme mass

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

protons

Be

Li He

neutrons

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

⁵⁶Ni neutron spectral function



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



Ab-Initio SCGF approaches



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...

(ph)

(ph)

O^{II}(pp/hh)

= hole

R^{(2p1}

= 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

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

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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:

 $\Sigma_{ab}^{11\,(1)} = \qquad \stackrel{a}{\overset{o}{b}} - - - \stackrel{c}{\overset{o}{d}} \bigcirc \downarrow \omega'$ $\Sigma_{ab}^{12\,(1)} = \qquad \stackrel{a}{\overset{c}{}} - - - \stackrel{\overline{b}}{\overset{d}{}} \stackrel{\overline{b}}{\overset{d}{}}$ UNIVERSITY OF



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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	







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:



- → Use if effective interactions
- Need to correct the Koltun sum rule (for energy)

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).



% 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

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





⁵⁶Ni neutron spectral function



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



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)







Modern realistic nuclear forces



Chiral Nuclear forces - SRG evolved





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:1412.3002 [nucl-th] (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) SURREY N2LO (Λ = 400Mev/c) chiral 3N interaction evolved (2.0fm⁻¹)

Results for the oxygen chain

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



→ Single particle spectra slightly to spread and

→ systematic underestimation of radii



Spectroscopic Factors



Spectroscopic factors @ limits of stability



- *Challenged* by recent experiments

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- May be correlations or scattering analysis

Quenching of absolute spectroscopic factors



Z/N asymmetry dependence of SFs - Theory

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

Effects of continuum become important at the driplines



Z/N asymmetry dependence of SFs - Theory

Ab-initio calculations explain the Z/N dependence but the effect is much lower than observed

Effects of continuum become important at the driplines

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[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 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)	$C^2 S_{\text{th}}$ (SCGF)	R _s (SCGF)
14 O (<i>d</i> , <i>t</i>) 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)
$^{16}O(d, t)$ ^{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

Knockout & transfer experiments

* Neutron removal from proton- and neutron- Ar isotopes @ NSCL:

				(theo.)	(ex	pt.)	(ex	pt.)
Isotopes	lj^{π}	Sn(MeV)	ΔS (MeV)	SF(LB-SM)	SF(JLM + HF)	Rs(JLM + HF)	SF(CH89)	<i>Rs</i> (CH89)
³⁴ Ar	$s1/2^{+}$	17.07	12.41	1.31	0.85 ± 0.09	0.65 ± 0.07	1.10 ± 0.11	0.84 ± 0.08
³⁶ Ar	$d3/2^{+}$	15.25	6.75	2.10	1.60 ± 0.16	0.76 ± 0.08	2.29 ± 0.23	1.09 ± 0.11
⁴⁶ Ar	$f7/2^{-}$	8.07	-10.03	5.16	3.93 ± 0.39	0.76 ± 0.08	5.29 ± 0.53	1.02 ± 0.10

[Lee et al. 2010]

	Sn (MeV)	ΔS (MeV)	SF		
³⁴ Ar ³⁶ Ar	33.0 27.7	18.6 7.5	1.46 1.46	- Gorkov GF NN	$\Delta S = Sn - Sp$
⁴⁶ Ar	16.0	-22.3	5.88	-	
³⁴ Ar	22.4	15.5	1.56		
³⁶ Ar ⁴⁶ Ar	15.3 6.5	7.2 -15.7	1.54 6.64	Gorkov GF NN + 3N	

UNIVERSITY OF V.Somà, CB, et al, Eur. Phys. Jour.: Web. of Conf. 66, 02005 (2014).

Knockout & transfer experiments

* Neutron removal from proton- and neutron- Ar isotopes @ NSCL:



UNIVERSITY OF V.Somà, CB, et al, Eur. Phys. Jour.: Web. of Conf. 66, 02005 (2014).

Calcium isotopic chain

Ab-initio calculation of the whole Ca: induced and full 3NF investigated



→ induced and full 3NF investigated

- \rightarrow genuine (N2LO) 3NF needed to reproduce the energy curvature and S_{2n}
- \rightarrow N=20 and Z=20 gaps overestimated!

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→ Full 3NF give a correct trend but over bind!

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



Two-neutron separation energies predicted by chiral NN+3NF forces:



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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



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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 UNIVERSITY OF



Two-neutron separation energies predicted by chiral NN+3NF forces:



Lack of deformation due to quenched cross-shell quadrupole excitations

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

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

M. Rosenbusch, et al., PRL114, 202501 (2015)



Measurements @ ISOLTRAP

Theory tend to overestimate the gap at N=34, but overall good

→ <u>Error bar in predictions</u> are from extrapolating the manybody expansion to convergence of the model space.



Inversion of $d_{3/2}$ — $s_{1/2}$ at N=28



FIG. 1. (color online) Experimental energies for $1/2^+$ and $3/2^+$ states in odd-A K isotopes. Inversion of the nuclear spin is obtained in ^{47,49}K and reinversion back in ⁵¹K. Results are

> J. Papuga, et al., Phys. Rev. Lett. 110, 172503 (2013); Phys. Rev. C 90, 034321 (2014)

> > 51

53

^AK isotopes Laser spectroscopy @ ISOLDE

Change in separation described by chiral NN+3NF:



Study of nuclear interactions from Lattice QCD

In collaboration with:





Why should we investigate LQCD interactions?

It gives complimentary insight to the EFT approach:

Allows to approach physical interaction from heavy quark masses
(opposite direction than the chiral limit).
Can study implications of SU(3) limit.

No need to fit to experiment. No LEC constants.
Provides consistent interactions in the Hyperon sector.

- It is very fundamental approach (QCD), and an alternative to Chiral-EFT.

Challenges and limitations:

- Mostly LO terms of the NN force exploited so far (but being improved).
- Physical pion mass limit requires efforts (but underway).
- NNN only barely addressed.
- Strong short-range repulsion is a challenge to ab-initio approaches.





$$L = -\frac{1}{4}G^a_{\mu\nu}G^{\mu\nu}_a + \bar{q}\gamma^{\mu}(i\partial_{\mu} - gt^aA^a_{\mu})q - m\bar{q}q$$



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Vacuum expectation value $\langle O(\bar{q}, q, U) \rangle \qquad \text{path integral} \\
= \int dU d\bar{q} dq e^{-S(\bar{q}, q, U)} O(\bar{q}, q, U) \\
= \int dU \det D(U) e^{-S_{U}(U)} O(D_{\uparrow}^{-1}(U)) \\
= \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} O(D^{-1}(U_{i})) \qquad \text{quark propagator}$

{ U_i } : ensemble of gauge conf. U generated w/ probability det $D(U) e^{-S_U(U)}$

Well defined (reguralized) * Fully non-perturvative
 Manifest gauge invariance * Highly predictive

Slide, courtesy of T. Inoue (see Oct. 8th talk)

Q

HAL Method

S. Aoki, T. Hatsuda, N. Ishii, Prog. Theo. Phys. 123 89 (2010) N. Ishii etal. [HAL QCD coll.] Phys. Lett. B712 , 437 (2012)

NBS wave function $\varphi_{\vec{k}}(\vec{r}) = \sum_{\vec{x}} \langle 0|B_i(\vec{x}+\vec{r},t)B_j(\vec{x},t)|B=2,\vec{k} \rangle$

Define a common potential U for all E eigenstates by a "Schrödinger" eq.

$$\left[-\frac{\nabla^2}{2\mu}\right]\varphi_{\vec{k}}(\vec{r}) + \int d^3\vec{r}' U(\vec{r},\vec{r}')\varphi_{\vec{k}}(\vec{r}') = E_{\vec{k}}\varphi_{\vec{k}}(\vec{r})$$

Non-local but energy independent below inelastic threshold

Measure 4-point function in LQCD

$$\psi(\vec{r},t) = \sum_{\vec{x}} \langle 0|B_i(\vec{x}+\vec{r},t)B_j(\vec{x},t)J(t_0)|0\rangle = \sum_{\vec{k}} A_{\vec{k}} \varphi_{\vec{k}}(\vec{r})e^{-W_{\vec{k}}(t-t_0)} + \cdots$$

$$\left[2M_B - \frac{\nabla^2}{2\mu}\right]\psi(\vec{r},t) + \int d^3\vec{r}'U(\vec{r},\vec{r}')\psi(\vec{r}',t) = -\frac{\partial}{\partial t}\psi(\vec{r},t)$$

 $\begin{array}{l} \nabla \text{ expansion} \\ \& \text{ truncation} \end{array} \quad U(\vec{r},\vec{r}\,') = \delta(\vec{r}-\vec{r}\,')V(\vec{r},\nabla) = \delta(\vec{r}-\vec{r}\,')[V(\vec{r})+\nabla+\nabla^2..] \end{array}$

Therefor, in the leading

$$V(\vec{r}) = \frac{1}{2\mu} \frac{\nabla^2 \psi(\vec{r},t)}{\psi(\vec{r},t)} - \frac{\frac{\partial}{\partial t} \psi(\vec{r},t)}{\psi(\vec{r},t)} - 2M_B$$
²⁷

Slide, courtesy of T. Inoue (see Oct. 8th talk)

HAL Method

Advantages:

- ✓ No need to separate E eigenstate. Just need to measure $\psi(\vec{r}, t)$
- \checkmark Then, potential can be extracted.
- ✓ Demand a minimal lattice volume. No need to extrapolate to V=∞.
- ✓ Can output more observables.
- ✓ One can address large nuclei too!!





Pictures, courtesy of T. Inoue (see Oct. 8th talk)

Two-Nucleon HAL potentials



- Left: NN potentials in partial waves at the lightest m_q .
 - Repulsive core & attractive pocket & strong tensor force.
 - Similar to phenomenological potentials qualitatively. e.g. AV18
 - Least χ^2 fit of data which give central value of observable.
 - Higher orders in velocity expansions are not available yet. We restrict us to these leading order potentials.
- Right: Quark mass dependence of V(r) of NN ¹S₀.
- Potentials become stronger as *m*q decrease.

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Two-Nucleon HAL potentials



- Quark mass dependence of potentials in NN ³S₁
- All components get bigger as quark mass decrease.



Application of microscopic (Ab-Initio) SCGF to potentials with hard cores.

How do we do it?? \rightarrow With a G-matrix!



Analysis of Brueckner HF

Scattering of two nucleon in free space:



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):



Different levels of approximation:



Sensitivity of BHF of the $\varepsilon(k)$ spectrum



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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Benchmark on ⁴He



→ Can expect accuracy on binding energies at about 10%

¹H. Nemura *et al.*, Int. J. Mod. Phys. E **23**, 1461006 (2014) ²H. Kamada *et al.*, Phys. Rev. C**64** 044001 (2001).



Binding of ¹⁶O and ⁴⁰Ca:



Binding energies are ~15 MeV ¹⁶O and 70-75MeV for ⁴⁰Ca. Possibly being underestimated by 10%

 \rightarrow 16O at m_{π}= 469 MeV is unstable toward 4- α breakup!

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Spectral strength in ¹⁶O and ⁴⁰Ca:



D SUKKEY

Matter distribution of ¹⁶O and ⁴⁰Ca:



→ Radii discrepancy worsens with increasing A









PNM unbound as usual, but less stiff

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SNM saturates at 469 MeV but under bound and at higher densities that physical.

T. Inoue et al., Phys. Rev. Lett. 111 112503 (2013).



SCGF in infinite SNM @ m_{π} =469MeV



Conclusions

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 deteriorate for medium mass isotopes (Ca and above) with roughly 1 MeV/A over binding.

HALQCD Nuclear forces:

- → Approaching the physical pion mass quickly
- → Strong short range repulsion requires new ideas in ab-initio many-body methods. Diagram resummation through G-matrix is a workable approach (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).



NNLO-sat : a global fit up to A≈24

A. Ekström et al. Phys. Rev. C91, 051301(R) (2015)



NNLOsat (V2 + W3) -- Grkv 2nd ord.

From SCGF:

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V2-N3LO(500) + W3-NNLO(400MeV/c) w/ SRG at 2.0 fm⁻¹
 A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013)
 V. Somà, CB *et al.* Phys. Rev. C**89**, 061301R (2014)

BE and charge radii in ^ACa



BE and charge radii in ^ACa





Similar quality of Ni isotopes

Up to A=78

