

CORTONA 2013 XIV CONVEGNO su PROBLEMI di FISICA NUCLEARE TEORICA

29-31 OTTOBRE 2013

Realistic shell-model calculations and exotic nuclei



Angela Gargano, INFN Napoli

Outline

- Theoretical framework
- Results for different mass regions
- ✓ Oxygen isotopes
- ✓ Nuclei north-east ⁴⁸Ca
- ✓ ¹³²Sn neighbors
- Outlook





• Eigenvalue problem

$$\mathbf{H}_{eff}\psi_{\alpha} = \mathbf{E}_{\alpha}\psi_{\alpha} \quad \mathbf{H}_{eff} = \mathbf{U} + \mathbf{V}_{eff} = \sum_{i} \varepsilon_{i} \mathbf{a}_{i}^{\dagger} \mathbf{a}_{i} + \frac{1}{4} \sum_{ijkl} \langle ij \mid \mathbf{V}_{eff} \mid kl \rangle \mathbf{a}_{i}^{\dagger} \mathbf{a}_{j}^{\dagger} \mathbf{a}_{k}$$





• Eigenvalue problem





• Eigenvalue problem

 Understand the properties of nuclei starting from the forces between nucleons

 Understand limits of the theory, because of the absence of free parameters





Schrödinger equation for A nucleons

$$\mathbf{H}\psi_{\alpha} = (\mathbf{H}_{0} + \mathbf{H}_{1})\psi_{\alpha} = \mathbf{E}_{\alpha}\psi_{\alpha} \begin{bmatrix} \mathbf{H}_{0} = \mathbf{T} + \mathbf{U} \\ \mathbf{H}_{1} = \mathbf{V}_{NN} - \mathbf{U} \end{bmatrix}$$





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Schrödinger equation for A nucleons

$$\mathbf{H}\psi_{\alpha} = (\mathbf{H}_{0} + \mathbf{H}_{1})\psi_{\alpha} = \mathbf{E}_{\alpha}\psi_{\alpha}$$

$$\mathbf{H}_{0} = \mathbf{T} + \mathbf{U}$$

$$\mathbf{H}_{1} = \mathbf{V}_{NN} - \mathbf{U}$$

Shell-model equation for N-valence nucleons in a

reduced space

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$$\mathbf{P}_{eff} \mathbf{P}_{\alpha} = \mathbf{P}_{\alpha} (\mathbf{H}_{0} + \mathbf{V}_{eff}) \mathbf{P}_{\alpha} = \mathbf{E}_{\alpha} \mathbf{P}_{\alpha} \psi_{\alpha}$$
$$\mathbf{P}_{\alpha} = \sum_{i=1}^{d} |\phi_{i}\rangle\langle\phi_{i}| \qquad \phi_{i} = [a_{1}^{+}a_{2}^{+}...a_{N}^{+}]|c\rangle$$

Derivation of H_{eff}

Two main ingredients

Nucleon-nucleon potential

Many-body theory

L. Coraggio et *al*, Prog. Part. Nucl. Phys. 62, 135 (2009) L. Coraggio et *al*, Annals of Phys. 327, 2061 (2012)





Nucleon-Nucleon potential

Potentials which reproduce the two-body data with $\chi^2/N_{data} \sim 1$



Chiral potentials

 ✓ long-range components ruled by the symmetries of the low-energy QCD

 ✓ two- and many-body forces generated on the same footing calculations: 2 body at next-to-next-to-next-to-leading order - N³LO
 3 body at next-to-next-to-leading order - NNLO





Optimitazion of the NN chiral potential

namely of the short-range components included as contact terms and parametrized in terms of constants

PRL 110,	192502 (201	3)
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PHYSICAL REVIEW LETTERS

week ending 10 MAY 2013

Optimized Chiral Nucleon-Nucleon Interaction at Next-to-Next-to-Leading Order

A. Ekström,^{1,2} G. Baardsen,¹ C. Forssén,³ G. Hagen,^{4,5} M. Hjorth-Jensen,^{1,2,6} G. R. Jansen,^{4,5} R. Machleidt,⁷
 W. Nazarewicz,^{5,4,8} T. Papenbrock,^{5,4} J. Sarich,⁹ and S. M. Wild⁹

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 ⁴Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA
 ⁵Department of Physics and Astronomy, University of Tennessee, Knowille, Tennessee 37996, USA
 ⁶Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824, USA
 ⁷Department of Physics, University of Idaho, Moscow, Idaho 83844, USA
 ⁸Faculty of Physics, University of Warsaw, ul. Hoža 69, 00-681 Warsaw, Poland
 ⁹Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA

We optimize the nucleon-nucleon interaction from chiral effective field theory at next-to-next-toleading order (NNLO). The resulting new chiral force NNLO_{opt} yields $\chi^2 \approx 1$ per degree of freedom for laboratory energies below approximately 125 MeV. In the A = 3, 4 nucleon systems, the contributions of three-nucleon forces are smaller than for previous parametrizations of chiral interactions. We use NNLO_{opt} to study properties of key nuclei and neutron matter, and we demonstrate that many aspects of nuclear structure can be understood in terms of this nucleon-nucleon interaction, without explicitly invoking three-nucleon forces.



V_{low-k} potential

High-momentum repulsive components of V_{NN} prevent its use in nuclear structure perturbative calculations

V_{low-k} potential

- is confined within a momentum-space cutoff $\boldsymbol{\Lambda}$

high-momentum modes are integrated out down to $\boldsymbol{\Lambda}$

 preserves the onshell properties of the original NN potential





The perturbative approach to the shell-model \mathbf{H}_{eff}

Q - box folded-diagram method

• H_{eff} is written as a series in terms of the $\hat{\mathbf{Q}}$ - box and its derivatives

$$\hat{\mathbf{Q}} = \mathbf{PH}_{\mathbf{1}}\mathbf{P} + \mathbf{PH}_{\mathbf{1}}\mathbf{Q} \frac{1}{\varepsilon - \mathbf{QHQ}}\mathbf{QH}_{\mathbf{1}}\mathbf{P}$$

Q=1-P

 $\varepsilon = unperturbed energy for a degenerate model space (PH₀P=<math>\varepsilon$)

 the series for H_{eff} is summed up by iterative techniques (Krenciglowa-Kuo, Lee-Suzuki)

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Diagrammatic expansion of the **Q**-box







Diagrammatic expansion of the Q-box



<u>Note:</u> No (V-U)-insertion diagrams [1-1+1-2] are shown except for the 1-body 1st-order case. These arise from the presence of -U in H₁=V-U, and are zero only when U=HF potential





Diagrammatic expansion of the $\hat{\mathbf{Q}}$ -box



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Modern calculations do not go beyond third order

Convergence properties

- order-by-order convergence
 - inclusion of diagrams up to finite order in the interaction

intermediate-state space convergence
 truncation of the Q space

L. Coraggio et al, Annals of Phys. 327, 2061 (2012)





Remarks on the calculation of $H_{\rm eff}$

H_{eff} is constructed for a two-valence-particle nucleus and used
 for more complex systems
 → three- or higher-body forces arising
 for these systems (even if the original potential contains only two-body
 terms) are not taken into account





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Single particle energies

$$H_{eff} = U + V_{eff} = U + V_{eff}^{(1)} + V_{eff}^{(2)}$$





Remarks on the calculation of H_{eff}



Oxygen isotopes

L. Coraggio et al, J.Phys, Conf. Ser. 312, 092021 (2011)

V_{eff} @ third order from N³LOW+ Coulomb interaction

N³LOW=N³LO with a sharp cutoff (2.1 fm⁻¹) \rightarrow no need of V_{low-k}

• SP energies from theory (S-box) for the neutron *sd* shell





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• SP energies from theory (S-box) for the neutron *sd* shell

magicity @ N= 14 & 16

location of the neutron drip line and 3-body forces

- T. Otsuka et al, PRL 105, 032501 (2010)
- G. Hagen et al, PRL 108, 242501 (2012)
- H. Hergert et al, PRL, 110, 242501 (2013)...

Yrast 2⁺ states in Oxygen isotopes







Ground-state energies for Oxygen isotopes



 Calculations overestimate the expt data: <u>fail to predict</u> <u>that ²⁶O e ²⁸O are unbound to two neutron decay</u>





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Three-body forces???





Nuclei north-east ⁴⁸Ca ₂₂Ti, ₂₄Cr, ₂₆Fe, and ₂₈Ni

- V_{eff} @ third order from V_{low-k} of CD-Bonn (Λ=2.6 fm⁻¹) + Coulomb interaction
- SP energies from experiment
- effective $e_{\pi} \& e_{\nu}$ derived consistently with H_{eff}



Interesting laboratory to study the shell evolution when adding neutrons \rightarrow long isotopic chains, *e.g* Fe and Ni





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Ni isotopes:

- ✓ N/Z value of 1.79 for 78 Ni
- ✓ the shell structure evolves through three different subshell closures at N = 28, 40, 50





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- Disappearance of the N=40 shell closure and onset of a collective behavior when removing protons from the f_{7/2} orbital
 "island of inversion" as @ N=20 (³²Mg)

S.M. Lenzi et al, PRC 82, 054301 (2010)
A. Gade et al, PRC 81, 051304(R) (2010)
K. Sieja et al, PRC 85,051301(R) (2012)...





• Ni isotopes:

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- Disappearance of the N=40 shell closure and onset of a collective behavior when removing protons from the f_{7/2} orbital "island of inversion" as @ N=20 (³²Mg)

This may be explained as due to the interplay of

- ✓ reduction in the neutron $g_{9/2}$ $f_{5/2}$ gap induced by proton holes in the $f_{7/2}$ orbital
- ✓ quadrupole-quadrupole component of the effective interaction between the neutron g_{9/2} and d_{5/2} orbitals

Energy of the yrast 2⁺ state and B(E2; 2⁺→0⁺) for Ca, Ti, Cr, Fe, and Ni @ N=40



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ESPE @ N=40

$$\overline{\varepsilon}_{j_{v}} = \varepsilon_{j_{v}} + \sum_{j_{\pi}} V^{M}(j_{v}j_{\pi}')N_{j}$$

$$V^{M} \text{ monopole interaction}$$

 N_i number of nucleons in orbit j



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Neutron ESPE @ N=40

 $\overline{\varepsilon}_{j_{v}} = \varepsilon_{j_{v}} + \sum_{j_{\pi}} V^{M}(j_{v}j_{\pi}')N_{j_{\pi}'}$ $V^{M} \text{ monopole interaction}$

 N_i number of nucleons in orbit j







Neutron ESPE @ N=40







Neutron ESPE @ N=40

Occupation numbers

\mathbf{J}_{v} \mathbf{J}_{v} \mathbf{J}_{π}			I	П
V ^M monopole interaction		πf7/2	1.87	1.69
v _j number of nucleons in orbit j	Ti	vg9/2	3.23	3.72
4 – N=40 isotones		vd5/2		0.36
$2 - d_{5/2}$		πf7/2	3.64	3.31
	Cr	vg9/2	2.88	3.73
-2 - g _{9/2}		vd5/2		0.57
$\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$		πf7/2	5.61	5.31
-6 p _{3/2} ~2.3 MeV	Fe	vg9/2	1.75	2.81
-8 ~ 5.0 MeV		vd5/2		0.33
-10		πf7/2	7.89	7.85
	Ni	vg9/2	0.42	0.47
20 22 24 20 20 Z		vd5/2		0.05
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 $\overline{\varepsilon}_{i} = \varepsilon_{i} + \sum V^{M}(j_{i}j_{j}')N_{i}$





A. Covello et *al*, J. Phys. Conf. Ser. **267**, 012019 (2011), and refs therein L. Coraggio et *al*, Phys. Rev. C **87**, 034309 (2013), and refs therein

• V_{eff} @ second order from V_{low-k} of CD-Bonn (Λ =2.2 fm⁻¹) + Coulomb interaction

• SP energies from experiment

proton particles and neutron holes in $0g_{7/2}$, 1d, 2s, $0h_{11/2}$ neutron particles in $0h_{9/2}$, 1f, 2p, $0i_{13/2}$







A. Covello et *al*, J. Phys. Conf. Ser. **267**, 012019 (2011), and refs therein L. Coraggio et *al*, Phys. Rev. C **87**, 034309 (2013), and refs therein

- V_{eff} @ second order from V_{low-k} of CD-Bonn (Λ =2.2 fm⁻¹) + Coulomb interaction
- SP energies from experiment

proton particles and neutron holes in $Og_{7/2}$, 1d, 2s, $Oh_{11/2}$ neutron particles in $Oh_{9/2}$, 1f, 2p, $Oi_{13/2}$

Possible changes of shell structure across the N=82 shell closure







Peculiar properties of ¹³⁴Sn and ¹³⁶Te; very low excitation energy of the yrast 2⁺ state

$\Delta = E_{exc}(2_{1}^{+})$	¹³⁴ Sn	¹³⁰ Sn	¹³⁴ Te	¹³⁶ Te
in MeV	0.73	1.22	1.28	0.61







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evidence for a quenching of the N=82 shell closure ?

or "neutron pairing reduction for N>82" ?







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evidence for a quenching of the N=82 shell closure ?

or "neutron pairing reduction for N>82" ?

The pairing force for 2 neutron particles in the 82-126 shell is significantly weaker than that

for 2 neutron holes or 2 proton particles in the 50-82 shell





Diagonal matrix elements of interaction for the $(vf_{7/2})^2$, $(\pi g_{7/2})^2$ and $(vh_{11/2})^{-2}$ configurations



Diagonal matrix elements of interaction for the $(vf_{7/2})^2$, $(\pi g_{7/2})^2$ and $(vh_{11/2})^{-2}$ configurations



Energy of the 2⁺,4⁺,6⁺ states for Sn isotopes







Energy of the 2⁺ state in Te isotopes







Energy of the 2⁺ state in Te isotopes



$$\begin{vmatrix} ^{132} \text{Te}; \mathbf{2}_{1}^{*} \end{pmatrix} = \mathbf{0.66} \begin{vmatrix} ^{134} \text{Te}; \mathbf{2}_{1}^{*} \\ \end{vmatrix} \begin{vmatrix} ^{130} \text{Sn}; \mathbf{0}_{gs}^{*} \end{pmatrix} + \mathbf{0.62} \begin{vmatrix} ^{134} \text{Te}; \mathbf{0}_{gs}^{*} \\ \end{vmatrix} \begin{vmatrix} ^{130} \text{Sn}; \mathbf{2}_{1}^{*} \\ \end{vmatrix} + \cdots$$

$$\begin{vmatrix} {}^{136} \operatorname{Te}; 2_{1}^{\scriptscriptstyle +} \\ \rangle = 0.72 \begin{vmatrix} {}^{134} \operatorname{Te}; & 0_{gs}^{\scriptscriptstyle +} \\ \end{vmatrix} \begin{vmatrix} {}^{134} \operatorname{Sn}; & 2_{1}^{\scriptscriptstyle +} \\ \rangle + 0.36 \begin{vmatrix} {}^{134} \operatorname{Te}; & 2_{1}^{\scriptscriptstyle +} \\ \end{vmatrix} \begin{vmatrix} {}^{134} \operatorname{Sn}; & 0_{gs}^{\scriptscriptstyle +} \\ \rangle + \cdots \end{vmatrix}$$





e _v =0.7 e	B(E2; $2^+ \rightarrow 0^+$) in W.u.				
e _π -1.55 e	Expt	Calc			
¹³⁰ Sn	1.2(3)	1.4			
¹³⁴ Sn	1.4(2)	1.6			
¹³⁰ Te	10(1)	7.8			
¹³⁴ Te	5.6(6)	4.9			
¹³⁶ Te	5.9(9)	9.9			

Expt from NP A 746, 83c (2004); NP A 752, 264c (2005); PRC 84, 061306(R) (2011)





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Evolution of the single-particle states around ¹³²Sn

How proton and neutron SP states change when adding pairs of neutrons and protons to ¹³³Sb and ¹³³Sn



One-particle spectroscopic factors which give direct information on single-particle excitations





Evolution of the single-particle states around 132**Sn**

How proton and neutron SP states change when adding pairs of neutrons and protons to ¹³³Sb and ¹³³Sn

One-particle spectroscopic factors which give direct information on single-particle excitations



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single-proton states

¹³⁷ Sb	E Calc
7/2+	0.0
5/2+	0.18
3/2+	0.33
1/2+	0.40
11/2-	2.59

single-neutron states

E Calc	C ² S Calc	E Expt	C ² S Expt
0.0	0.86	0.0	0.94
0.73	0.57	0.60	0.52
1.13	0.43	0.98	0.35
1.33	0.72	1.22	0.43
1.35	0.17	1.30	0.22
2.08	0.75	1.75	0.84
	E Calc 0.0 0.73 1.13 1.33 1.35 2.08	E CalcC2S Calc0.00.8600.730.5771.130.4331.330.7221.350.1772.080.755	E CalcC ² S CalcE Expt0.00.8600.00.730.5770.6001.130.4330.9831.330.7221.221.350.1771.3002.080.7551.755

		sir	igle-pr	oton s	states	th	¹³⁷ Sb
	¹³⁷ S	b	E Calc			oton streng	g _{7/2}
	7/2+		0.0			- - - -	d
	5/2+		0.18			d sing	<u> </u>
	3/2+		0.33			0.4 -	n _{11/2}
	1/2+		0.40			nS 0.2-	d _{3/2}
	11/2-		2.59				s _{1/2}
	si	ngl	e-neu	tron st	tates	0.0	1 2 3 4 5 6 7 8 9 10 11 12 13 14 number of states
		-	020	-	020		¹³⁷ Xe
137	د ر	E alc	C ² S Calc	E Expt	C ² S Expt	1 ⁻ ج	f _{7/2}
7/2-	0.	0	0.86	0.0	0.94	8,0 g	h _a /a
3/2-	0.	73	0.57	0.60	0.52	6,0 tron	P ₂ /2
1/2-	1.	13	0.43	0.98	0.35	nəu- ə 0,4	P1/2
9/2-	1.	33	0.72	1.22	0.43	l singl	• 1/2
5/2-	1.	35	0.17	1.30	0.22	0,2 E	f _{5/2}
12/7	± 2	00	0.75	1 75	0 0 1	0 S r	

Restoration of the N = 82 Shell Gap from Direct Mass Measurements of ^{132,134}Sn

M. Dworschak,^{1,*} G. Audi,² K. Blaum,^{1,3,4} P. Delahaye,⁵ S. George,^{1,3} U. Hager,⁶ F. Herfurth,¹ A. Herlert,⁵ A. Kellerbauer,⁴ H.-J. Kluge,^{1,7} D. Lunney,² L. Schweikhard,⁸ and C. Yazidjian¹

0.5 MeV deviation from the accepted value restores the neutron shell gap at N=82 considered to be a case of "shell quenching"

PRL 109, 032501 (2012)

PHYSICAL REVIEW LETTERS

week ending 20 JULY 2012

Precision Mass Measurements beyond ¹³²Sn: Anomalous Behavior of Odd-Even Staggering of Binding Energies

J. Hakala,* J. Dobaczewski, D. Gorelov, T. Eronen,[†] A. Jokinen, A. Kankainen, V. S. Kolhinen, M. Kortelainen, I. D. Moore, H. Penttilä, S. Rinta-Antila, J. Rissanen, A. Saastamoinen, V. Sonnenschein, and J. Äystö[‡] Department of Physics, P.O. Box 35 (YFL), FI-40014 University of Jyväskylä, Finland (Received 5 March 2012; published 16 July 2012)

Atomic masses of the neutron-rich isotopes $^{121-128}$ Cd, 129,131 In, $^{130-135}$ Sn, $^{131-136}$ Sb, and $^{132-140}$ Te have been measured with high precision (10 ppb) using the Penning-trap mass spectrometer JYFLTRAP. Among these, the masses of four *r*-process nuclei 135 Sn, 136 Sb, and 139,140 Te were measured for the first time. An empirical neutron pairing gap expressed as the odd-even staggering of isotopic masses shows a strong quenching across N = 82 for Sn, with a Z dependence that is unexplainable by the current theoretical models.





$$\Delta^{(3)}(N,Z) = \frac{1}{2} [B(N+1,Z) + B(N-1,Z) - 2B(N,Z)]$$

self-consistent calculations with SLy4 Skyrme energy density functional + contact pairing force



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$$\Delta^{(3)}(N,Z) = \frac{1}{2} [B(N+1,Z) + B(N-1,Z) - 2B(N,Z)]$$



L. Coraggio et al, PRC 88, 041301(R) 2013)







• The drop of 0.5 MeV in the observed OES for Sn when crossing N = 82 is accounted for by the different pairing properties of V_{eff} for neutron particles and neutron holes

• When going to Te and Xe, the N = 81 and 83 lines **come closer to each other as a result of the** *p-n* V_{eff} . (*repulsive in the particle-hole channel, attractive in the particle-particle channel*). The two lines would be parallel should one ignore this interaction: **L. Coraggio et al, PRC 88, 041301(R) 2013**)





Binding energies relative to ¹³²Sn of Sn, Sb,Te, Xe

Nucleus	B_{calc}	B_{expt}
	$({ m MeV})$	$({ m MeV})$
134 Sn	5.98	6.03
135 Sn	8.37	8.30
$^{134}\mathrm{Sb}$	12.74	12.84
$^{135}\mathrm{Sb}$	16.32	16.58
$^{136}\mathrm{Sb}$	18.81	19.47
$^{134}\mathrm{Te}$	20.81	20.57
$^{135}\mathrm{Te}$	23.82	23.83
$^{136}\mathrm{Te}$	28.26	28.60
$^{137}\mathrm{Te}$	31.15	31.55
136 Xe	40.32	39.04
$^{137}\mathrm{Xe}$	43.83	43.06
$^{138}\mathrm{Xe}$	48.89	48.73

Expt from PRL 109,032501 (2012)





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$^{135}\mathrm{Te}$	23.82	23.83	
$^{136}\mathrm{Te}$	28.26	28.60	
$^{137}\mathrm{Te}$	31.15	31.55	
¹³⁶ Xe	40.32	39.04	
137 Xe	43.83	43.06	
138 Xe	48.89	48.73	

Expt from PRL 109,032501 (2012)







Test of the optimized chiral potential

- Role of genuine and effective three-body forces
- Microscopic origin of the properties of the shell-model interaction
- Further studies of nuclei far from stability





Naples group

- L. Coraggio
- A. Covello
- **A. G.**
- N. Itaco

Grazie per l'attenzione



