The role of continuum and three-nucleon forces in neutron rich nuclei.

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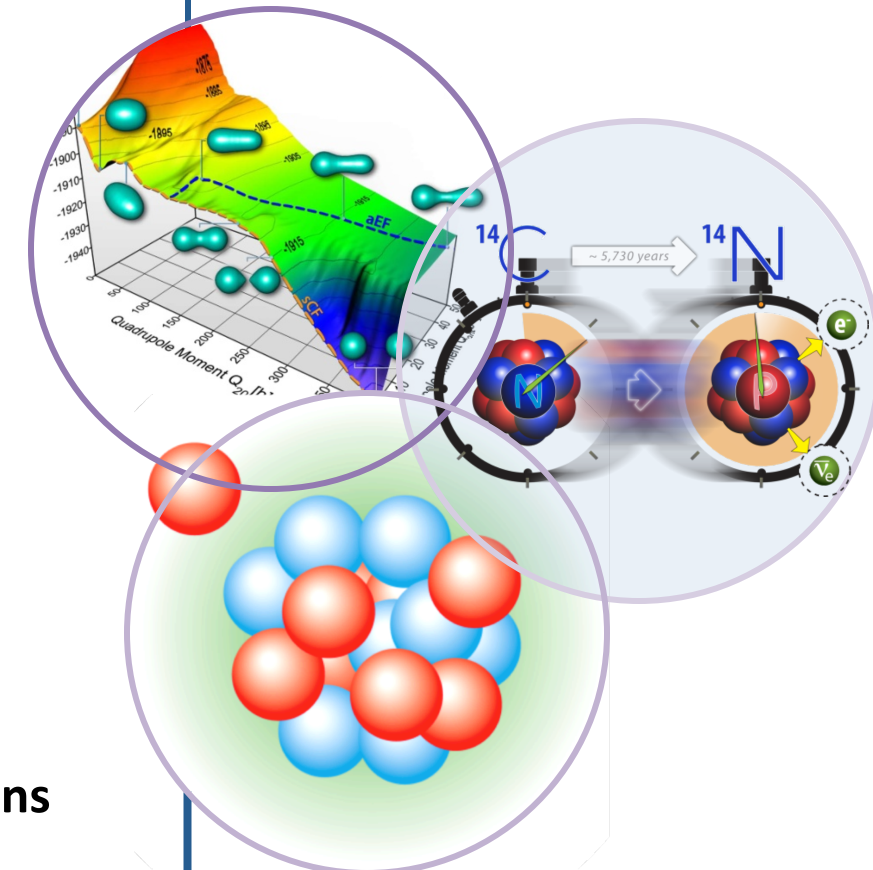


International Workshop XLI on Gross Properties of Nuclei and Nuclear Excitations

Hirschegg, January 29, 2013

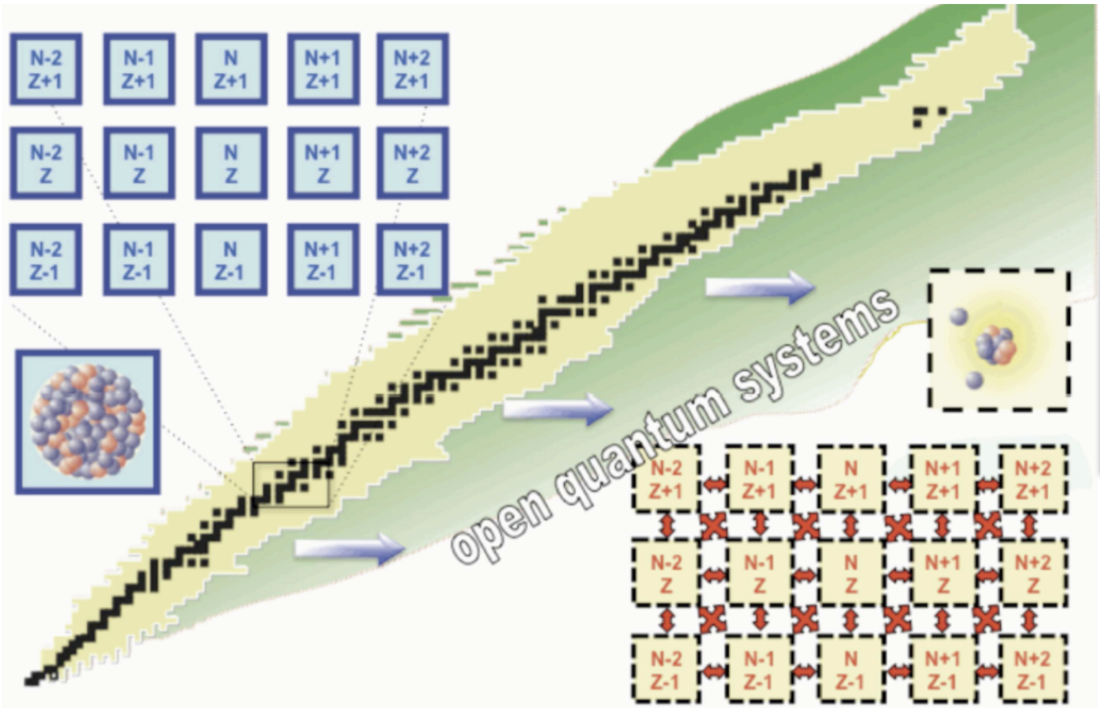
U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Outline

1. Open-quantum systems: how to describe physics of nuclei at the edge of stability?
2. Interactions from chiral EFT and Coupled-Cluster theory
3. Evolution of shell structure in neutron rich calcium isotopes – Is ^{54}Ca a magic nucleus?
4. Shell evolution in Potassium isotopes
5. Role of continuum and three-nucleon forces in neutron rich oxygen and fluorine isotopes
6. Proton elastic scattering of ^{40}Ca using CC
7. Computing scattering obersvables from a finite Harmonic oscillator basis

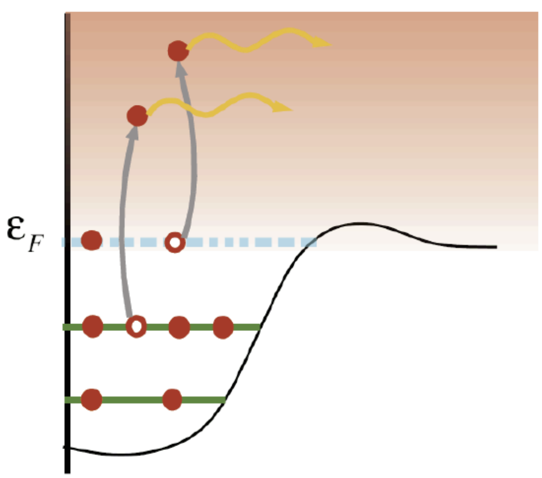
Physics of nuclei at the edges of stability

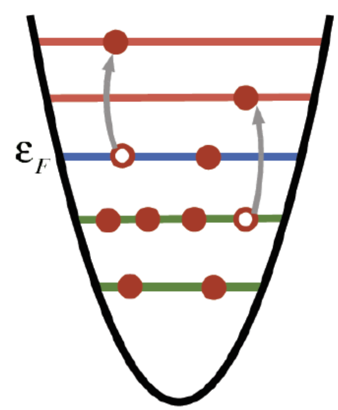


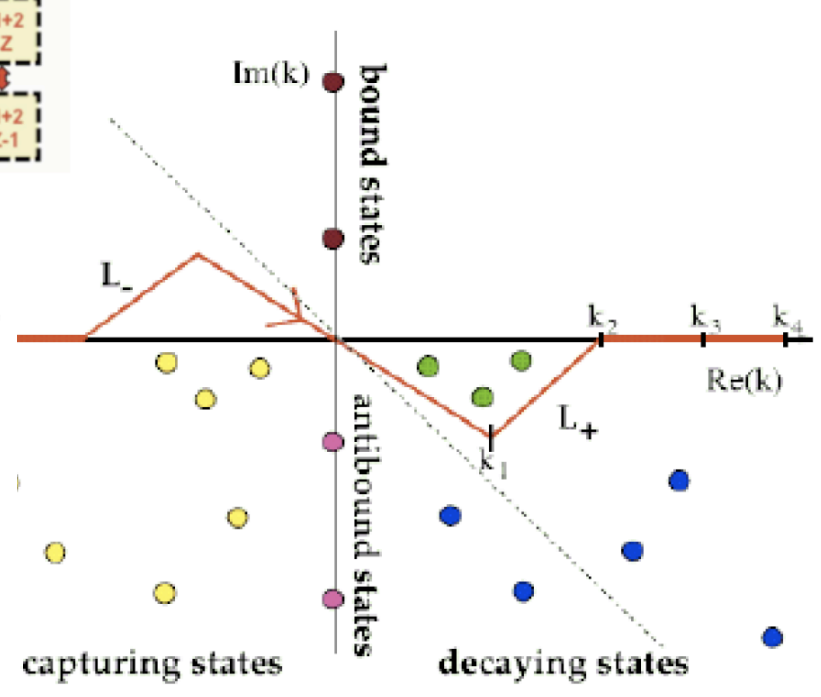
The Berggren completeness treats bound, resonant and scattering states on equal footing.

Has been successfully applied in the shell model in the complex energy plane to light nuclei. For a review see

N. Michel et al J. Phys. G 36, 013101 (2009).

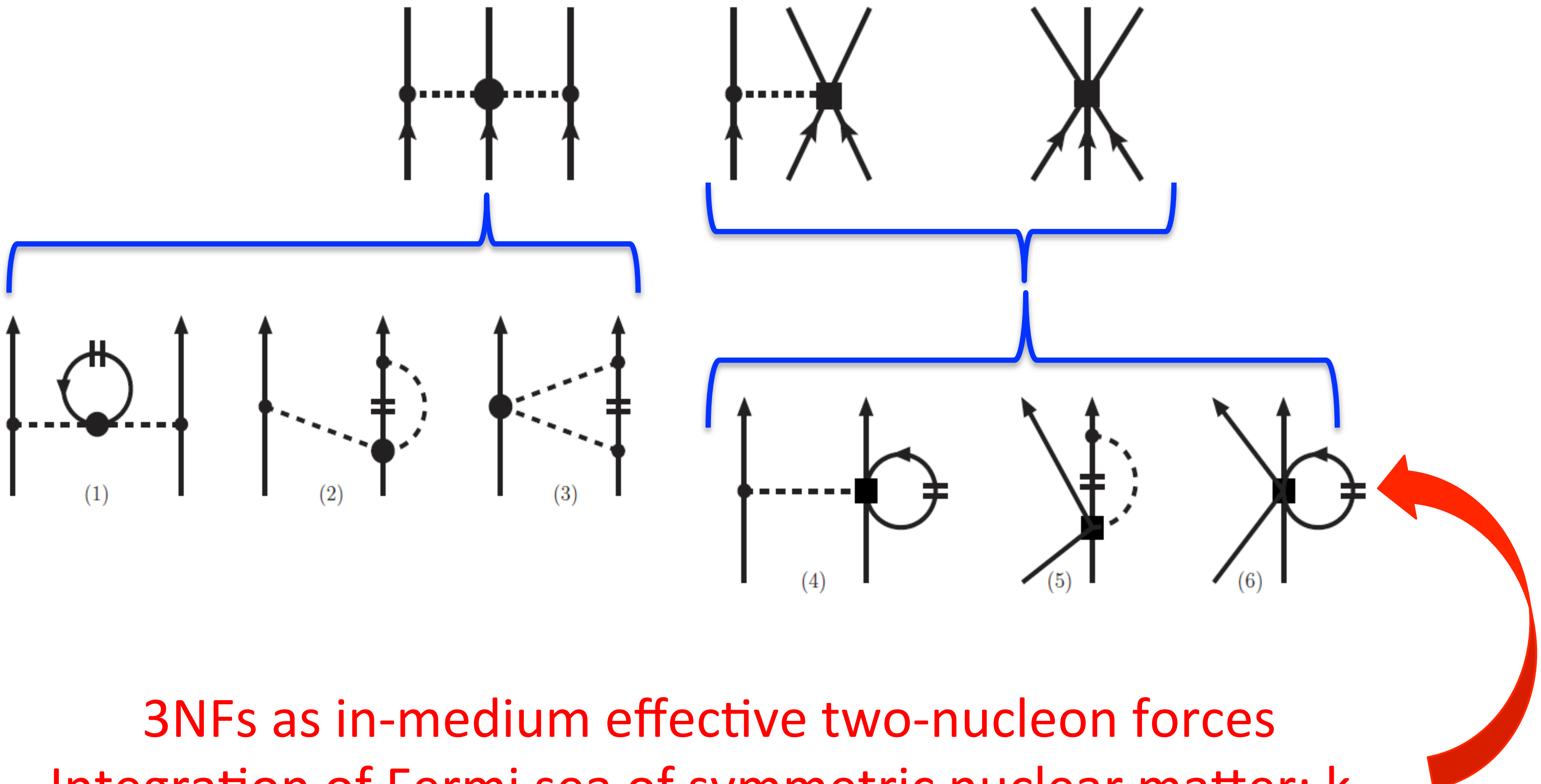






Including the effects of 3NFs (approximation!)

[J.W. Holt, Kaiser, Weise, PRC 79, 054331 (2009); Hebeler & Schwenk, PRC 82, 014314 (2010)]



3NFs as in-medium effective two-nucleon forces

Integration of Fermi sea of symmetric nuclear matter: k_F

Parameters: For Oxygen we use k_F=1.05 fm^{-1}, c_E=0.71, c_D=-0.2 from binding energies of $^{16,22}O$, for Calcium we use k_F = 0.95 fm^{-1}, c_E = 0.735, c_D = -0.2 from binding energy of ^{48}Ca and ^{52}Ca (The parameters c_D, c_E differ from values proposed for light nuclei)

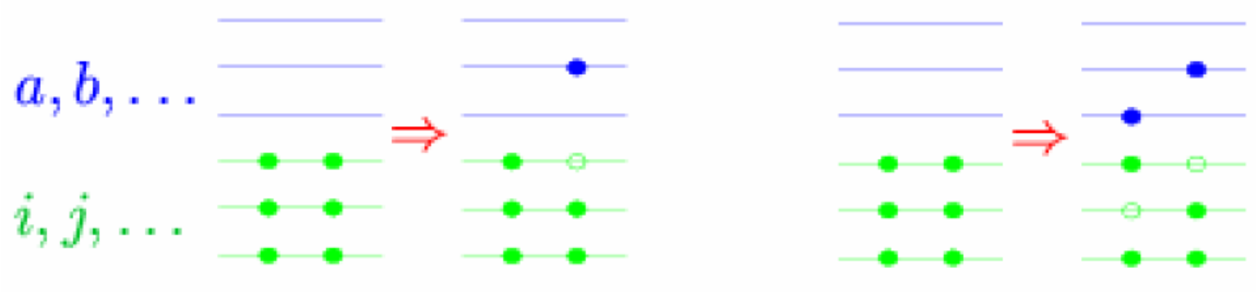
Coupled-cluster method (in CCSD approximation)

Ansatz:

$$
\begin{aligned}
|\Psi\rangle &= e^T|\Phi\rangle \\
T &= T_1 + T_2 + \ldots \\
T_1 &= \sum_{ia} t_i^a a_a^\dagger a_i \\
T_2 &= \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i
\end{aligned}
$$

- ☺ Scales gently (polynomial) with increasing problem size o^2u^4 .
- ☺ Truncation is the only approximation.
- ☺ Size extensive (error scales with A)
- ☹ Most efficient for doubly magic nuclei

Correlations are *exponentiated* 1p-1h and 2p-2h excitations. Part of np-nh excitations included!

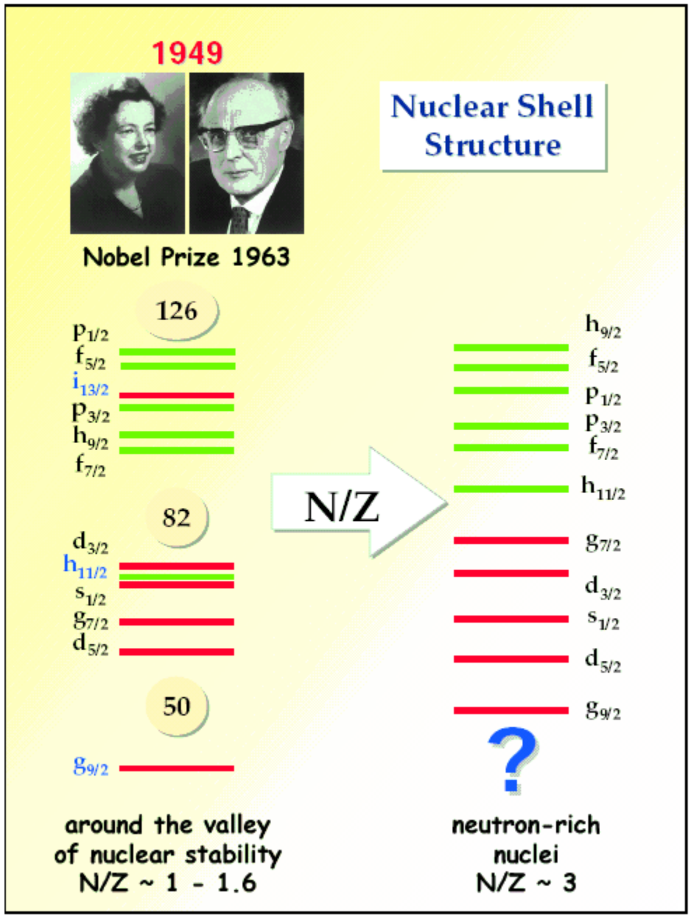


Coupled cluster equations

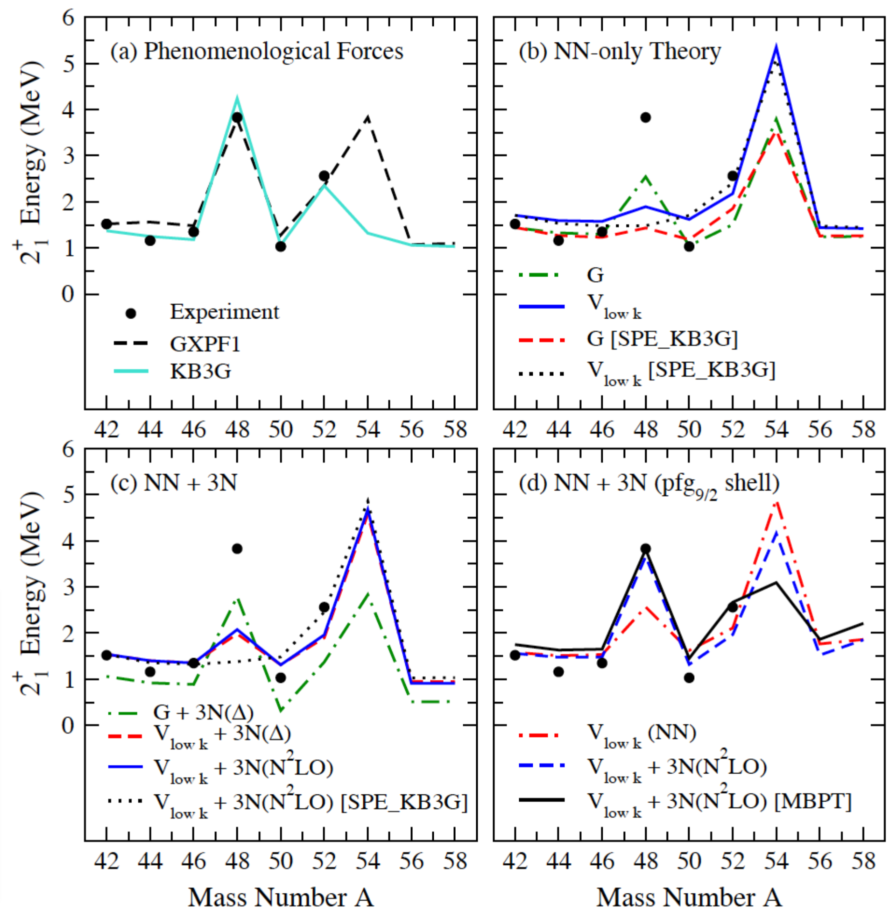
$$
\begin{aligned}
E &= \langle\Phi|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_i^a|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_{ij}^{ab}|\overline{H}|\Phi\rangle \\
\overline{H} &\equiv e^{-T}He^T = \left(He^T\right)_c = \left(H + HT_1 + HT_2 + \frac{1}{2}HT_1^2 + \ldots\right)_c
\end{aligned}
$$

Alternative view: CCSD generates similarity transformed Hamiltonian with no 1p-1h and no 2p-2h excitations.

Evolution of shell structure in neutron rich Calcium



- How do shell closures and magic numbers evolve towards the dripline?
- Is the naïve shell model picture valid at the neutron dripline?



- 3NFs are responsible for shell closure in ^{48}Ca
- Different models give conflicting result for shell closure in ^{54}Ca.

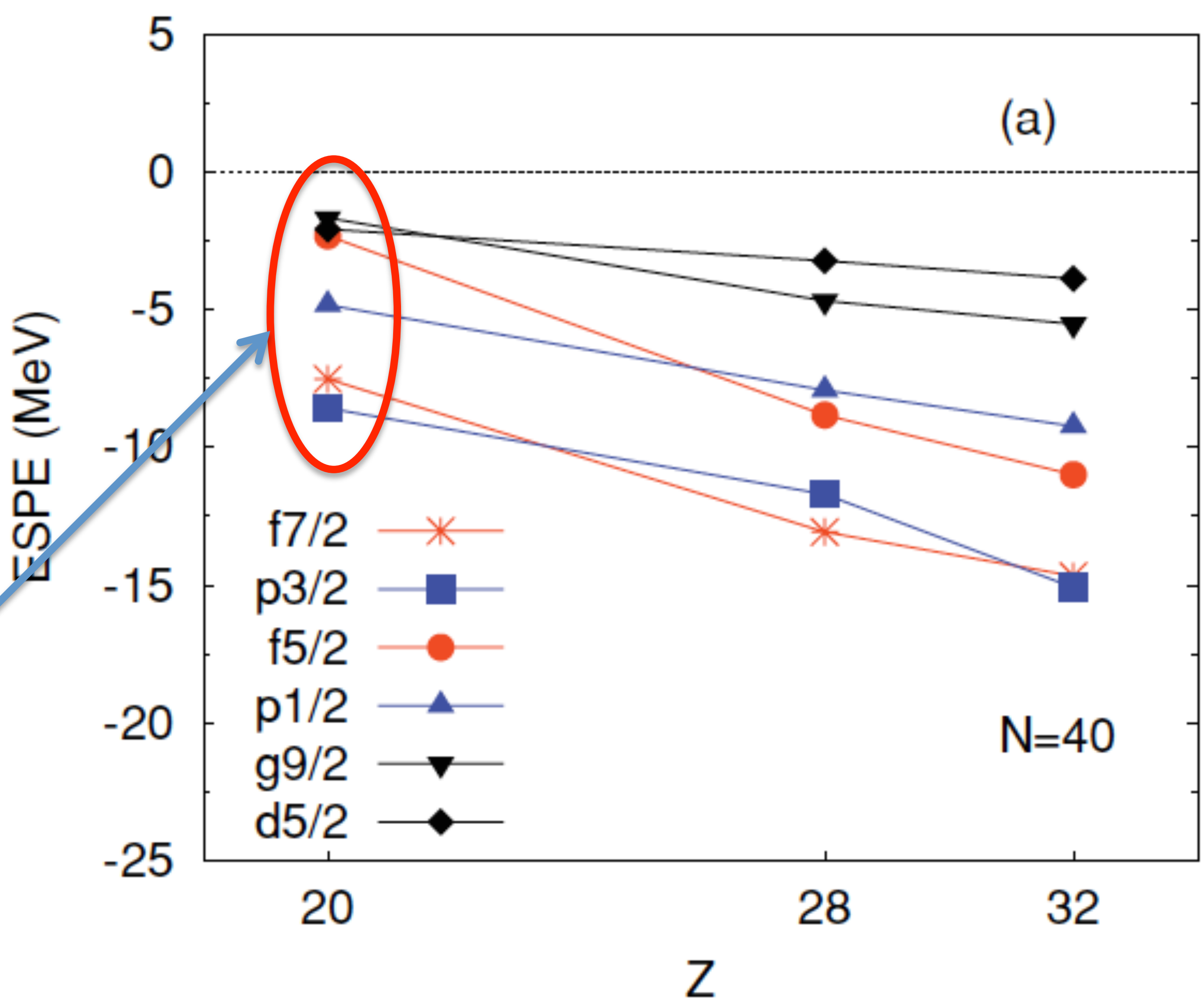
J. D. Holt et al, J. Phys. G **39**, 085111 (2012)

Evolution of shell structure in neutron rich Calcium

Inversion of shell order in ^{60}Ca

S. M. Lenzi, F. Nowacki, A. Poves, and K. Sieja Phys. Rev. C 82, 054301 (2010)

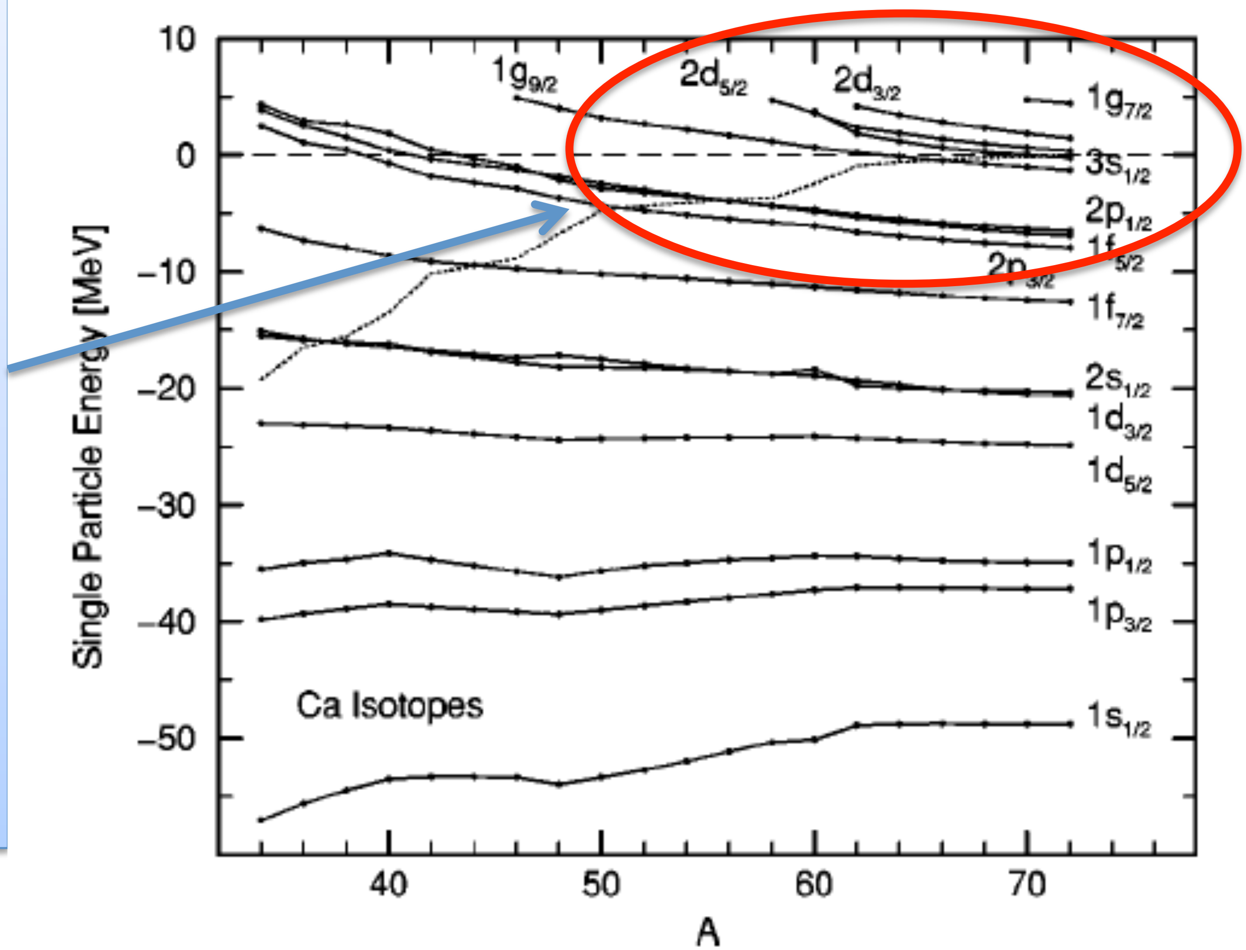
- Inversion of d5/2 and g9/2 in ^{60}Ca.
- Bunching of levels pointing to no shell-closure.



Evolution of shell structure in neutron rich Calcium

- Relativistic mean-field show no shell gap in $^{60-70}Ca$
- Bunching of single-particle orbitals
- large deformations and no shell closure

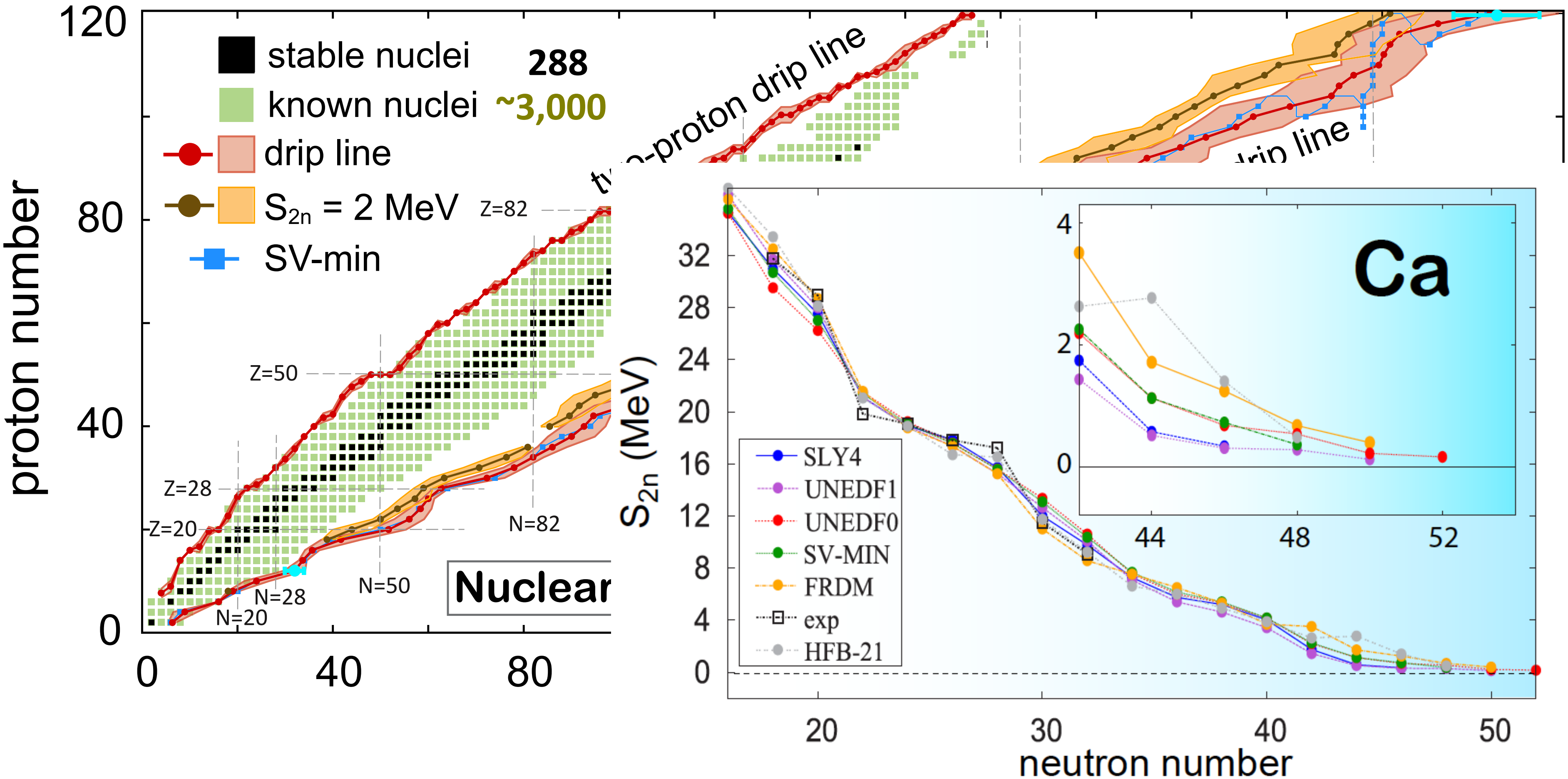
J. Meng et al, Phys. Rev. C 65, 041302(R) (2002)



How many protons and neutrons can be bound in a nucleus?

Literature: 5,000-12,000

Skyrme-DFT: 6,900±500$_{syst}$

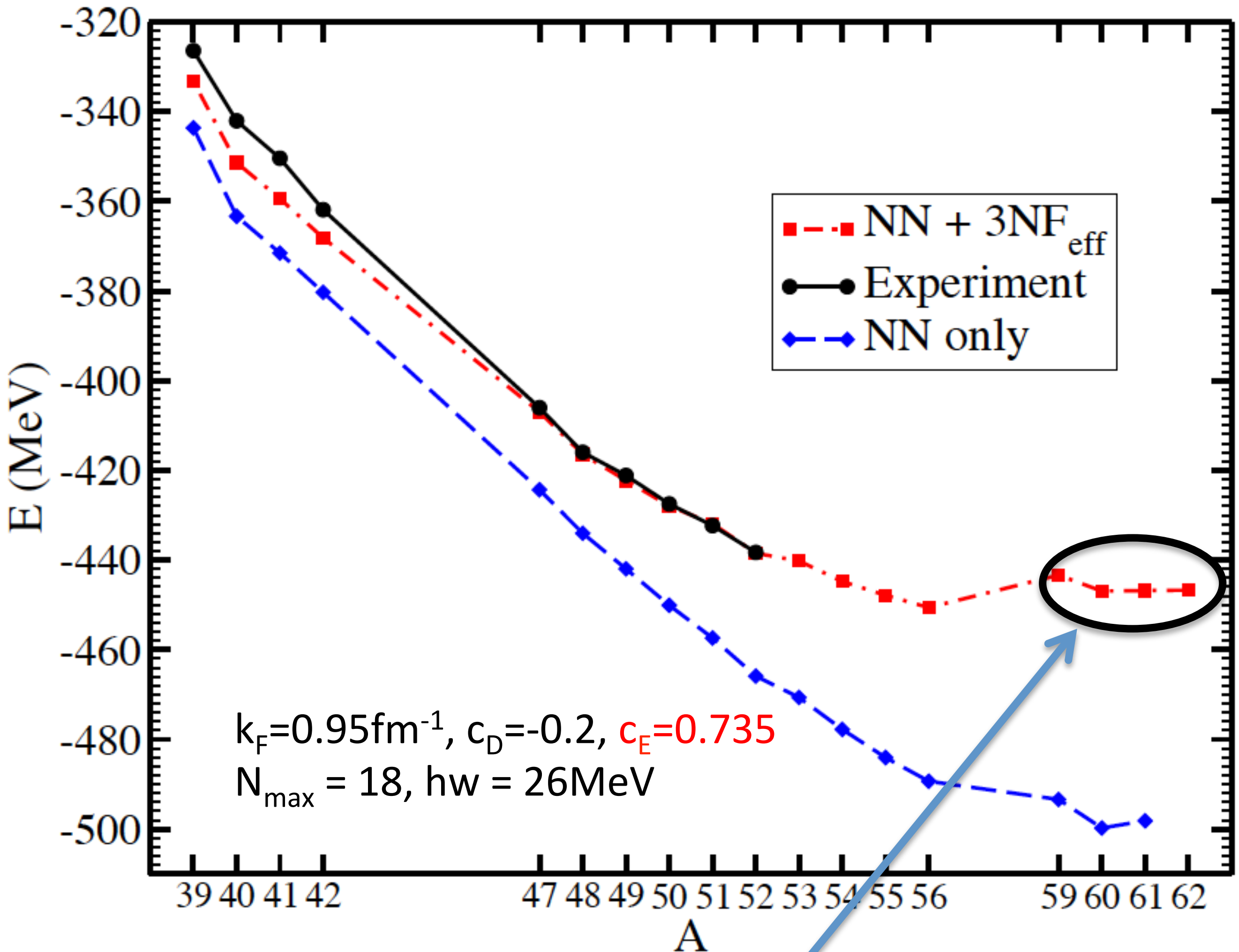


Description of observables and model-based extrapolation

- Systematic errors (due to incorrect assumptions/poor modeling)
- Statistical errors (optimization and numerical errors)

Erler et al., Nature 486, 509 (2012)

Calcium isotopes from chiral interactions



A peninsula of weak stability?

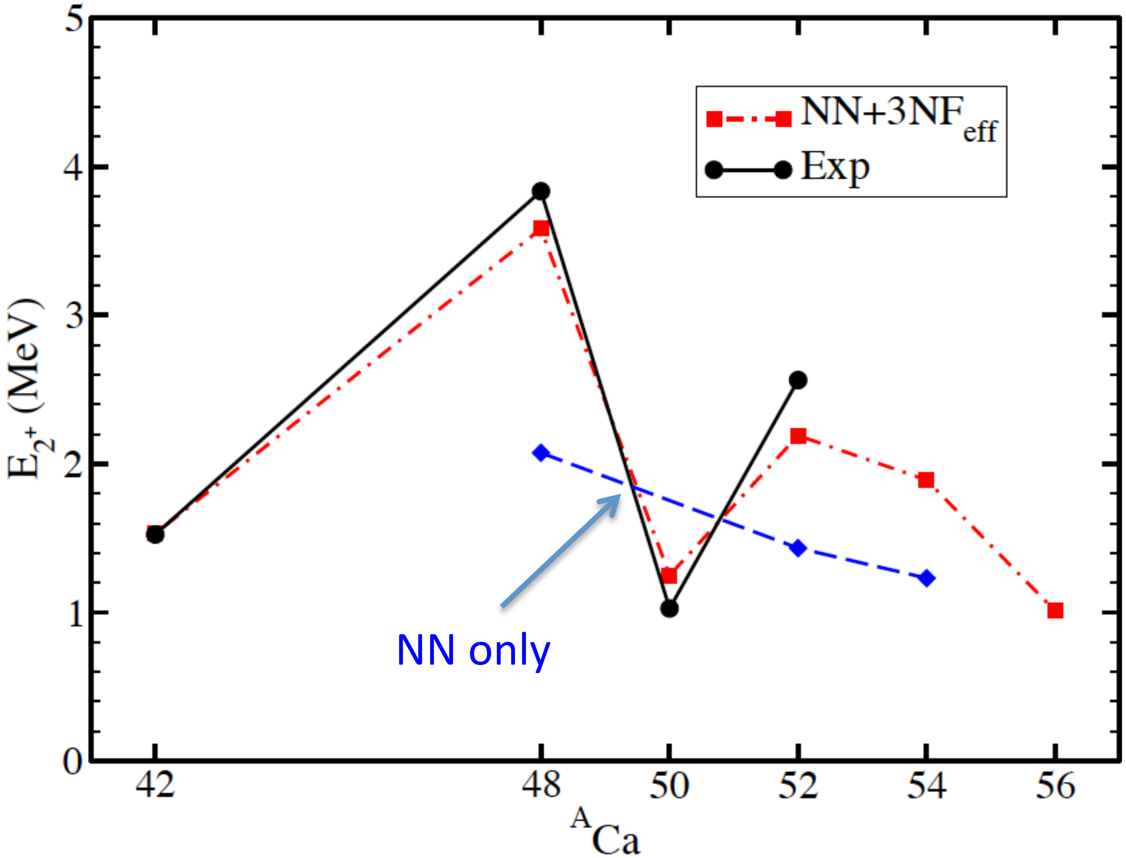
Main Features:

1. Total binding energies agree well with experimental masses.
2. Masses for $^{40-52}$Ca are converged in 19 major shells.
3. ^{60}Ca is not magic
4. $^{61-62}$Ca are located right at threshold.

<u>See also:</u>
Meng et al PRC 65, 041302 (2002), Lenzi et al PRC 82, 054301 (2010) and Erler et al, Nature 486, 509 (2012)

G. Hagen, M. Hjorth-Jensen, G. R. Jansen, R. Machleidt, T. Papenbrock, Phys. Rev. Lett. 109, 032502 (2012).

Is ^{54}Ca a magic nucleus? (Is N=34 a magic number?)



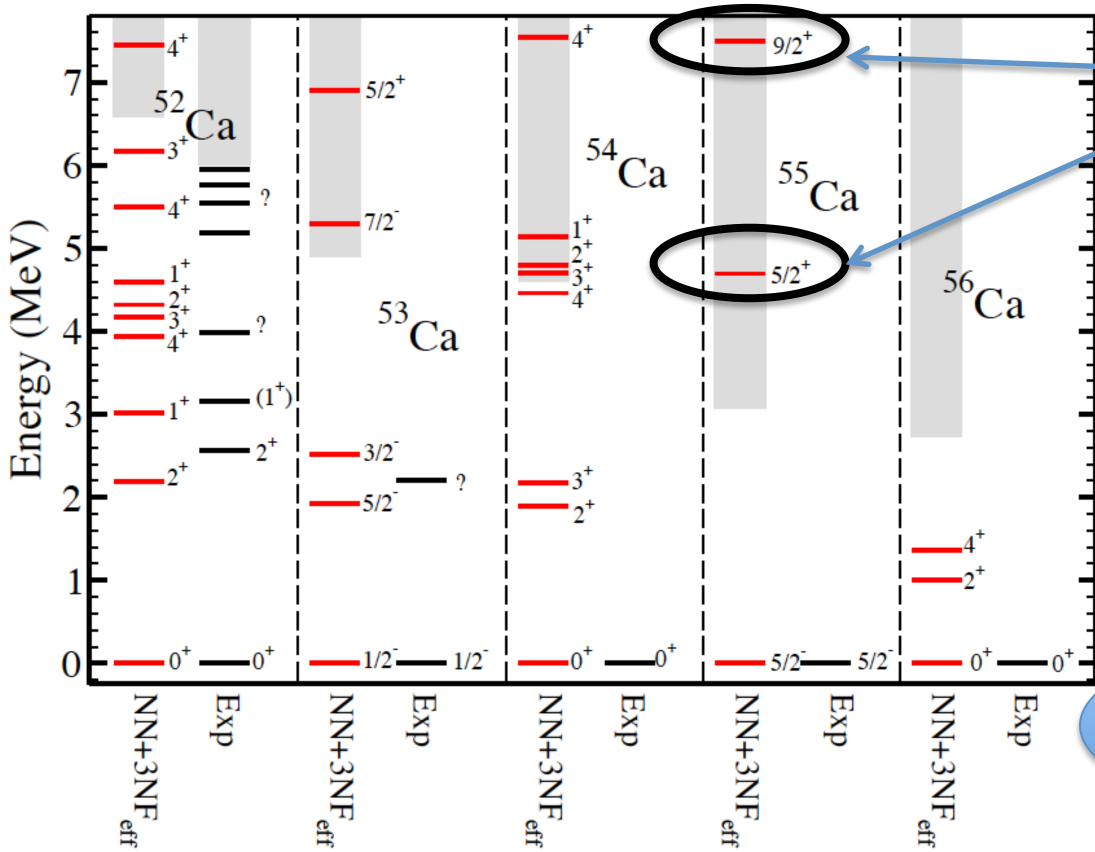
Main Features:

1. Good agreement between theory and experiment.
2. Shell closure in ^{48}Ca due to effects of 3NFs
3. Predict weak (sub-)shell closure in ^{54}Ca.

Hagen, Hjorth-Jensen, Jansen, Machleidt, T. Papenbrock, Phys. Rev. Lett. 109, 032502 (2012).

	^{48}Ca			^{52}Ca			^{54}Ca		
	2^+	4^+	$4^+/2^+$	2^+	4^+	$4^+/2^+$	2^+	4^+	$4^+/2^+$
CC	3.58	4.20	1.17	2.19	3.95	1.80	1.89	4.46	2.36
Exp	3.83	4.50	1.17	2.56	?	?	?	?	?

Spectra and shell evolution in Calcium isotopes



1. Inversion of the 9/2+ and 5/2+ resonant states in ^{53,55,61}Ca
2. We find the ground state of ^{61}Ca to be ½+ located right at threshold.
3. A harmonic oscillator basis gives the naïve shell model ordering of states.

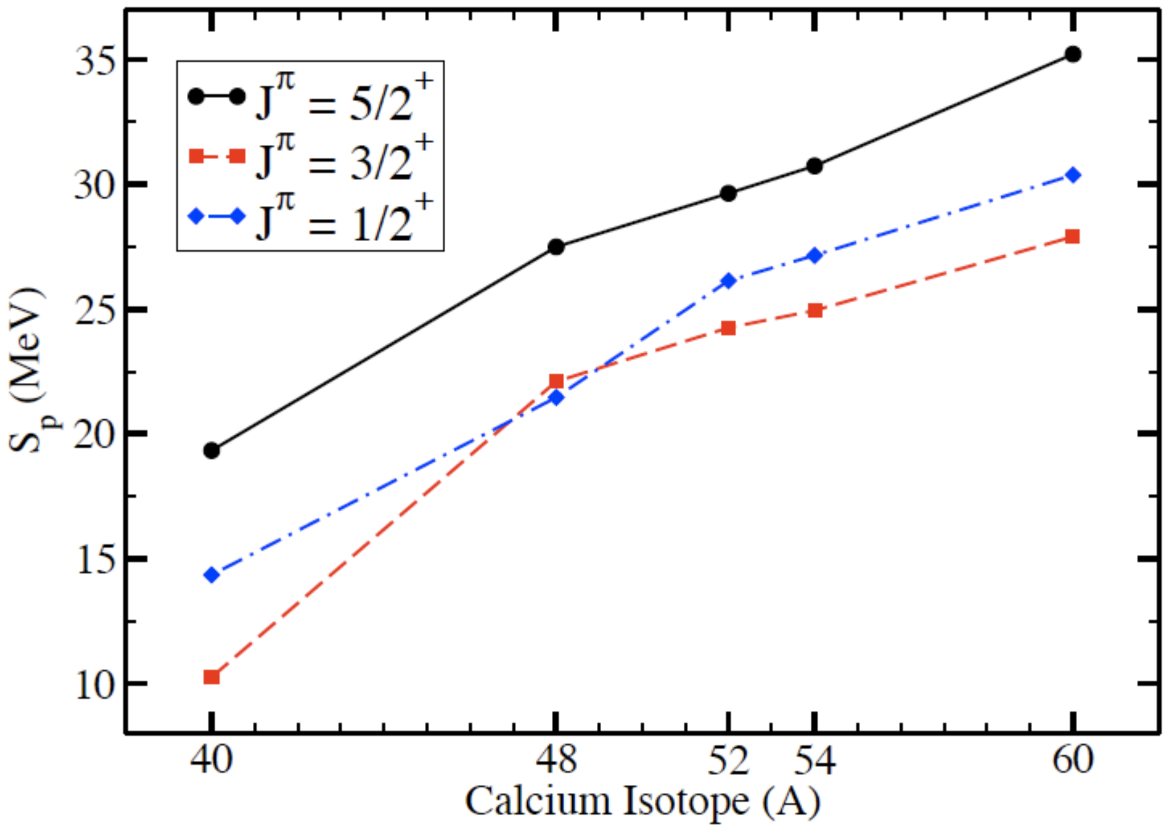
Continuum coupling is crucial!

	^{48}Ca	^{52}Ca	^{54}Ca
E_{2^+}(CC)	3.58	2.19	1.89
E_{2^+}(Exp)	3.83	2.56	n.a.
E_{4^+}/E_{2^+}(CC)	1.17	1.80	2.36
E_{4^+}/E_{2^+}(Exp)	1.17	n.a.	n.a.
S_n(CC)	9.45	6.59	4.59
S_n(Exp)	9.95	6.0*	4.0†

New penning trap measurement of masses of ^{51,52}Ca
A. T. Gallant et al Phys. Rev. Lett. **109**, 032506 (2012)

	^{53}Ca		^{55}Ca		^{61}Ca	
J^π	Re[E]	Γ	Re[E]	Γ	Re[E]	Γ
$5/2^+$	1.99	1.97	1.63	1.33	1.14	0.62
$9/2^+$	4.75	0.28	4.43	0.23	2.19	0.02

Evolution of the 3/2$^+$ and 1/2$^+$ states in Potassium

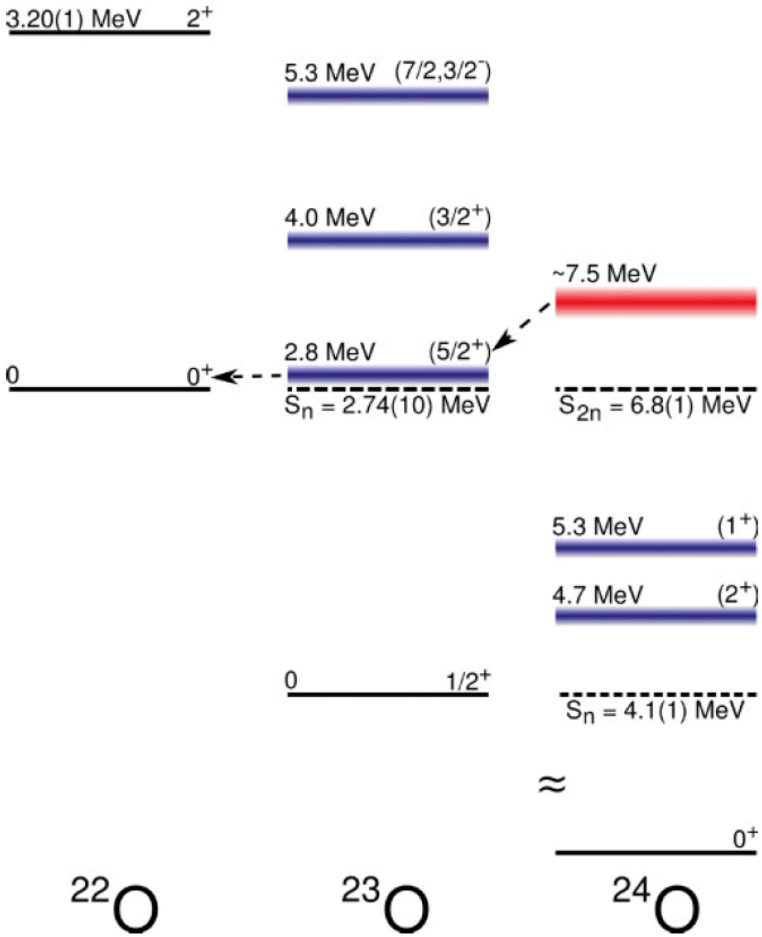


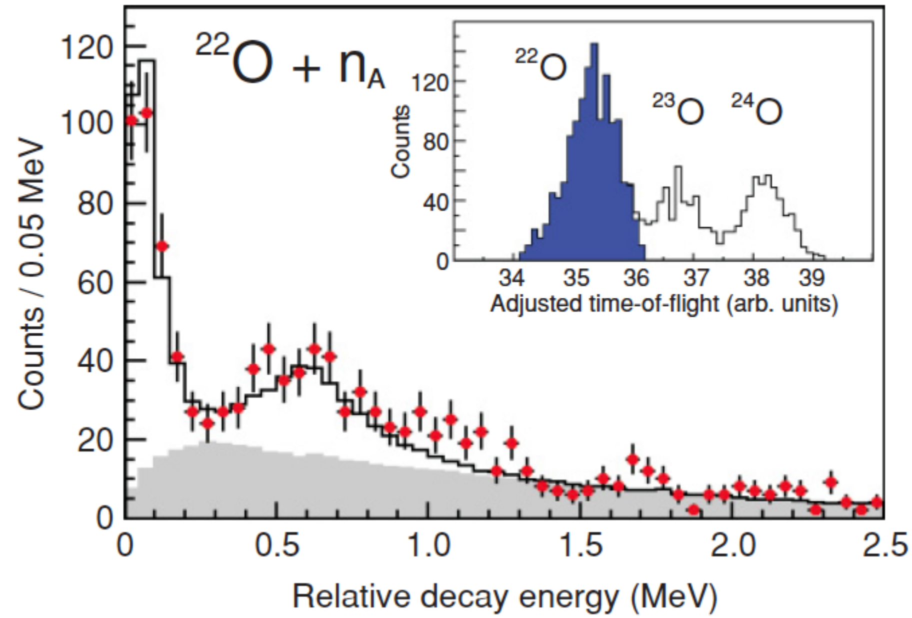
1. We reproduce level inversion in ^{47}K and get ½$^+$ as the ground state.
2. We predict 3/2$^+$ for the ground state in ^{51,53,59}K.

½$^+$ state with respect to 3/2$^+$ state in ^{39}K and ^{47}K.

	^{39}K		^{47}K	
J^π	E(CC)	E(Exp)	E(CC)	E(Exp)
3/2$^+$	0.00	0.00	0.00	0.00
1/2$^+$	4.097	2.52	-0.636	-0.36

Resonances in neutron rich oxygen-24

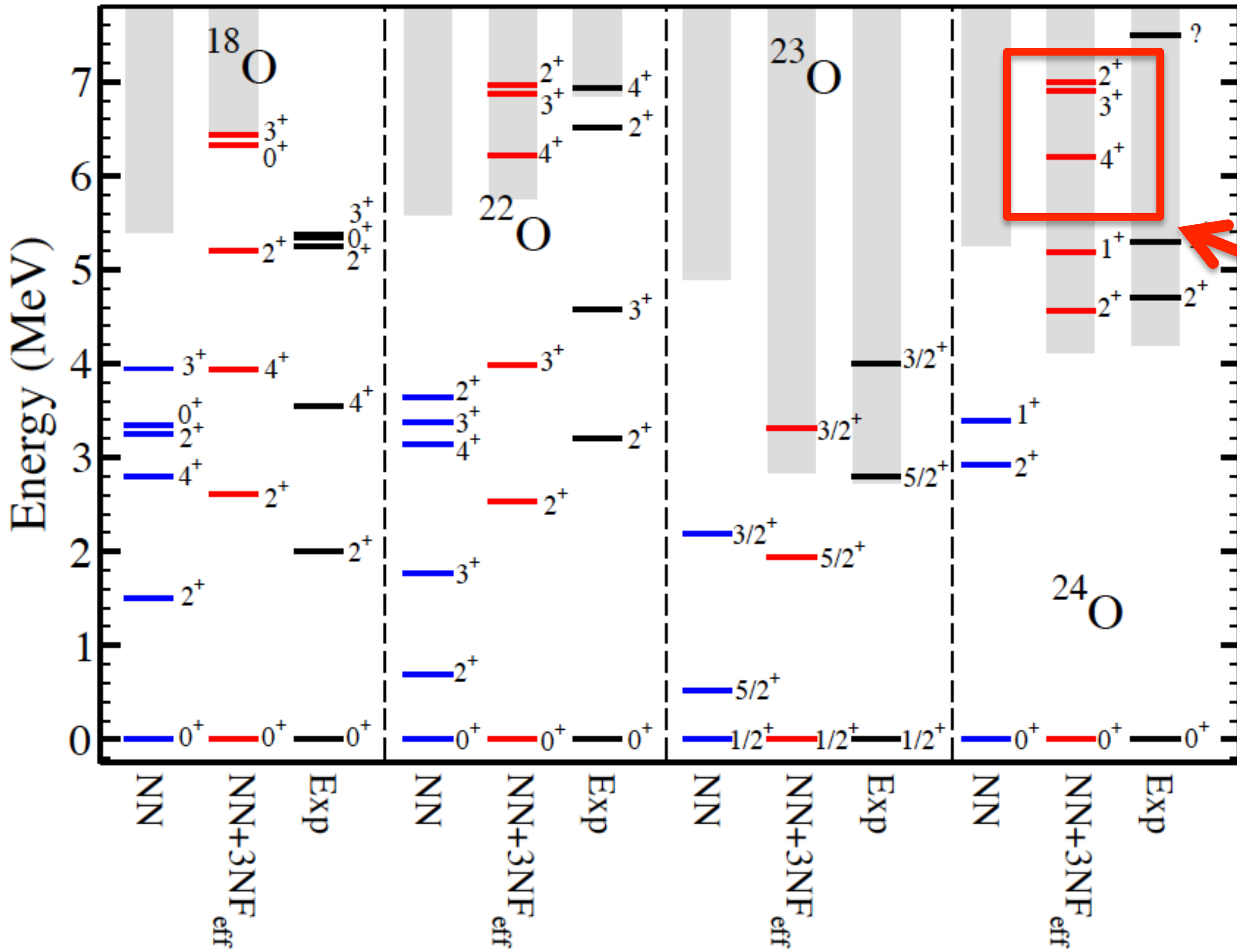




C. R. Hoffman et al Phys. Rev. C **83**, 031303(R) (2011)

- Knockout reaction of ^{26}F reveal a resonance above the two-neutron threshold in ^{24}O
- No spin and parity assigned of this state
- A challenge for microscopic theory to address these states

Oxygen isotopes from chiral interactions



The effects of three-nucleon forces decompress the spectra and brings it in good agreement with experiment.

We find several states (4^+,3^+,2^+) near the observed peak at ~7.5MeV in ^{24}O
C. R. Hoffman et al Phys. Rev. C **83**, 031303 (2011)

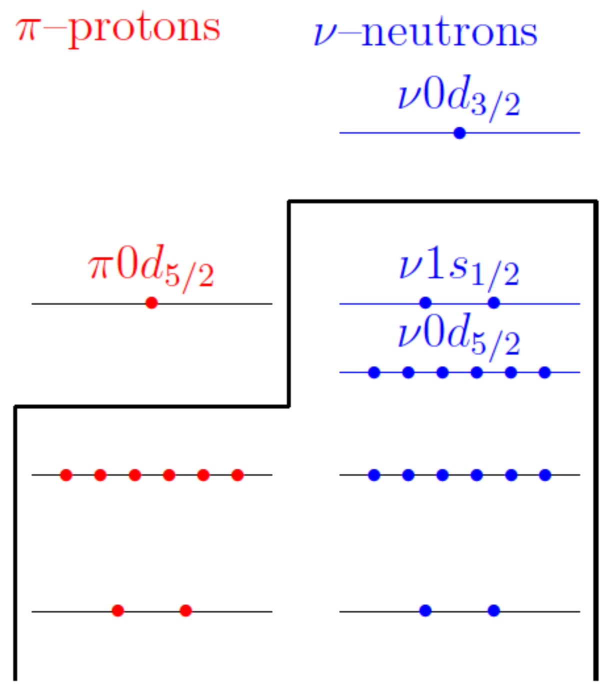
J^π	2_1^+	1_1^+	4_1^+	3_1^+	2_2^+	1_2^+
$E_{\rm CC}$	4.56	5.2	6.2	6.9	7.0	8.4
$E_{\rm Exp}$	4.7(1)	5.33(10)				
$\Gamma_{\rm CC}$	0.03	0.04	0.005	0.01	0.04	0.56
$\Gamma_{\rm Exp}$	$0.05^{+0.21}_{-0.05}$	$0.03^{+0.12}_{-0.03}$				

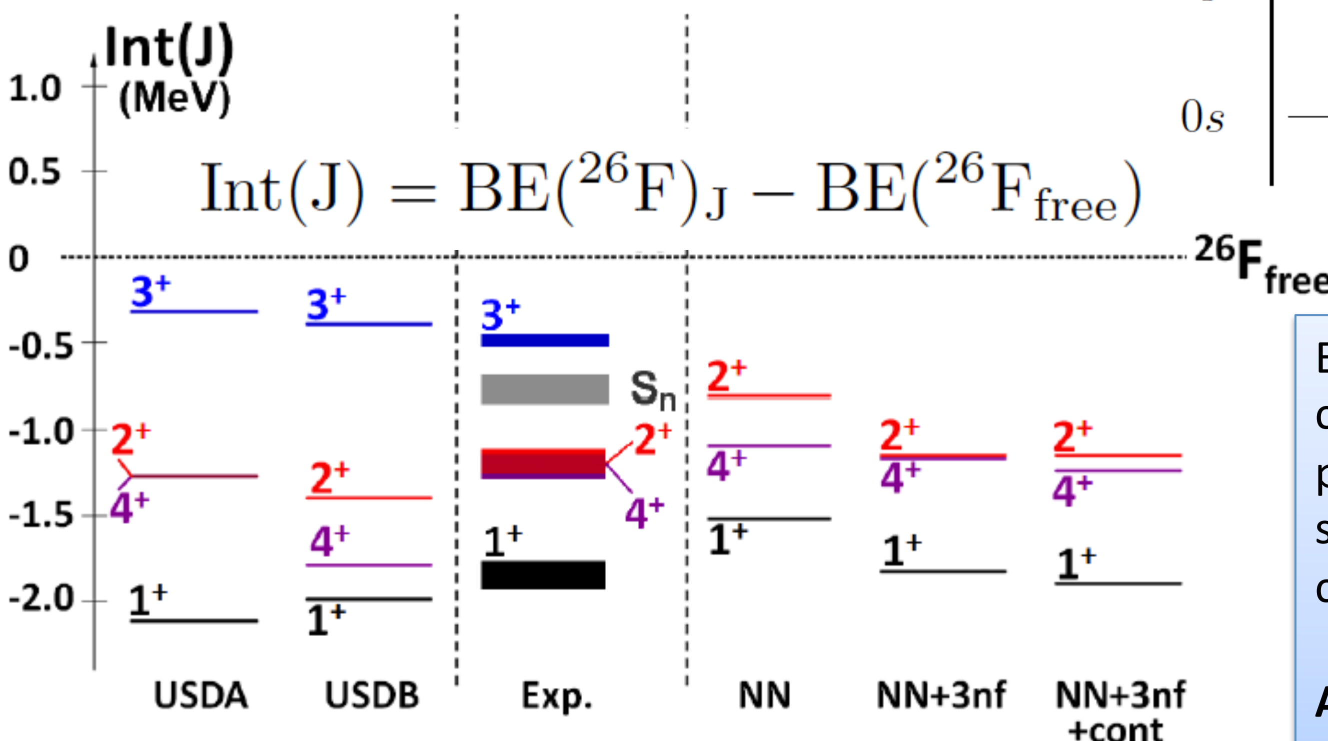
Hagen, Hjorth-Jensen, Jansen, Machleidt, T. Papenbrock, Phys. Rev. Lett. 108, 242501 (2012).

Computing open-shell Fluorine-26

$$(\bar{H}\hat{R}_\mu^{(A\pm2)})_C|\Phi_0\rangle = \omega_\mu \hat{R}_\mu^{(A\pm2)}|\Phi_0\rangle$$

$$\hat{R}^{(A+2)} = \frac{1}{2}\sum_{ba} r^{ab} a_a^\dagger a_b^\dagger + \frac{1}{6}\sum_{iabc} r_i^{abc} a_a^\dagger a_b^\dagger a_c^\dagger a_i + \dots$$

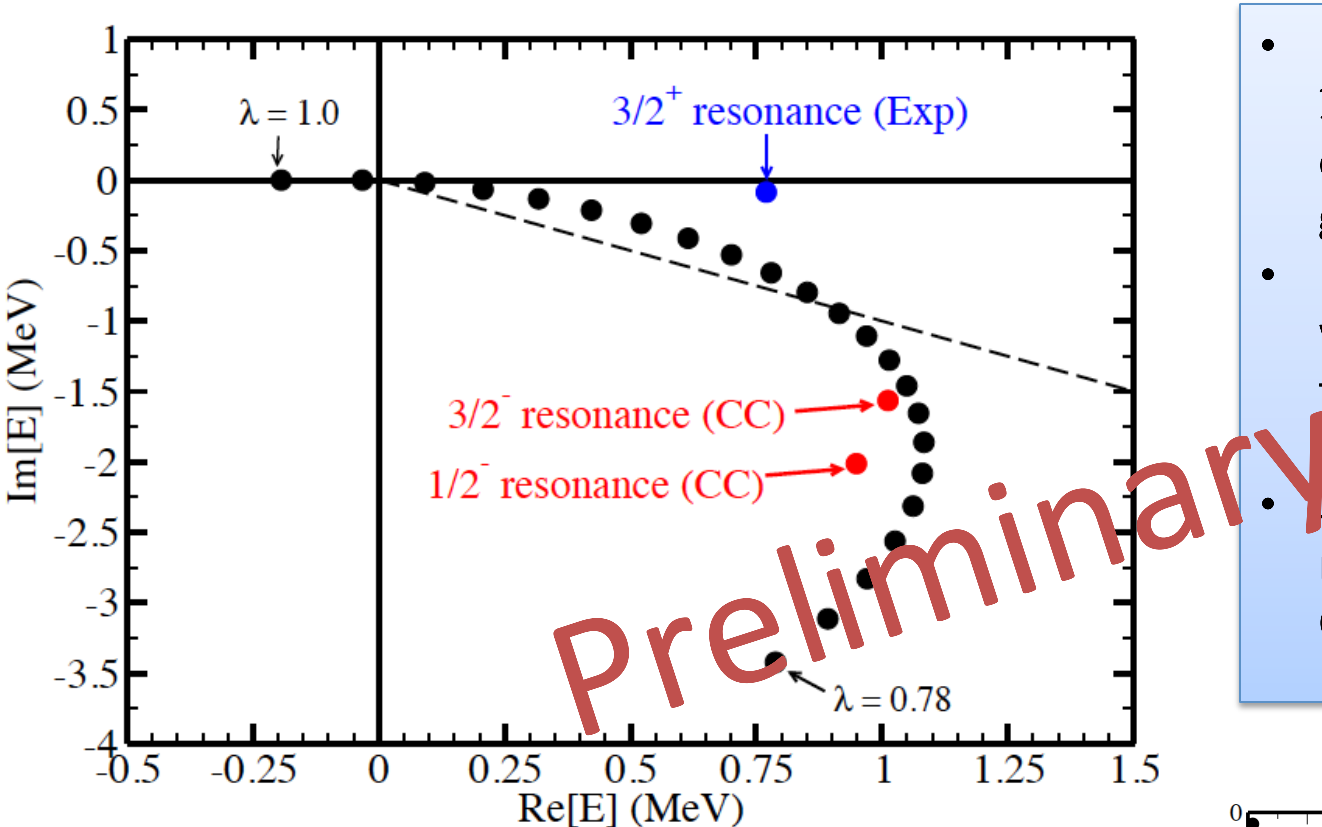




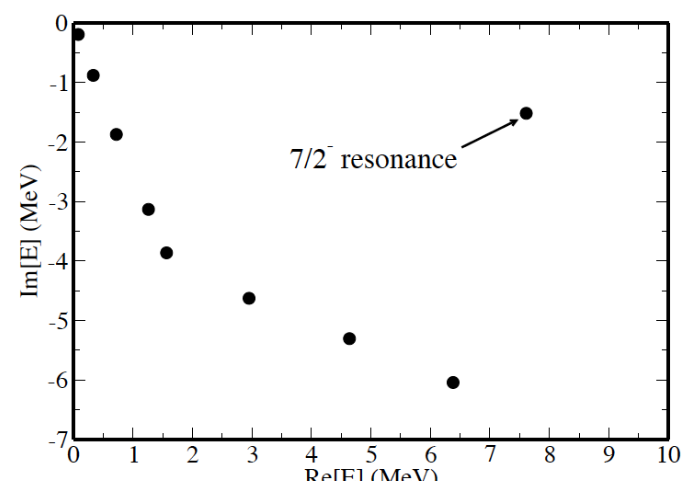
Experimental spectra in ^{26}F compared with phenomenological USD shell-model calculations and coupled-cluster calculations

A. Lepailleur et al, accepted for publication in PRL(2012)

Negative parity states in ^{25}O?



- Low-lying 3/2$^-$ and ½$^-$ intruder states close to the 3/2$^+$ groundstate in ^{25}O
- Due to very large width of these states they will be difficult to measure.
- Simple Woods-Saxon model agrees with CC results.

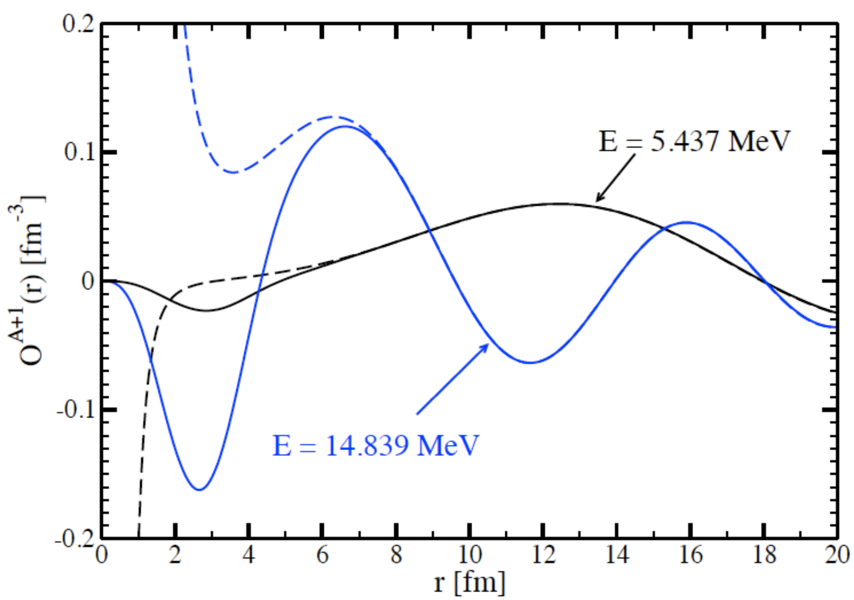


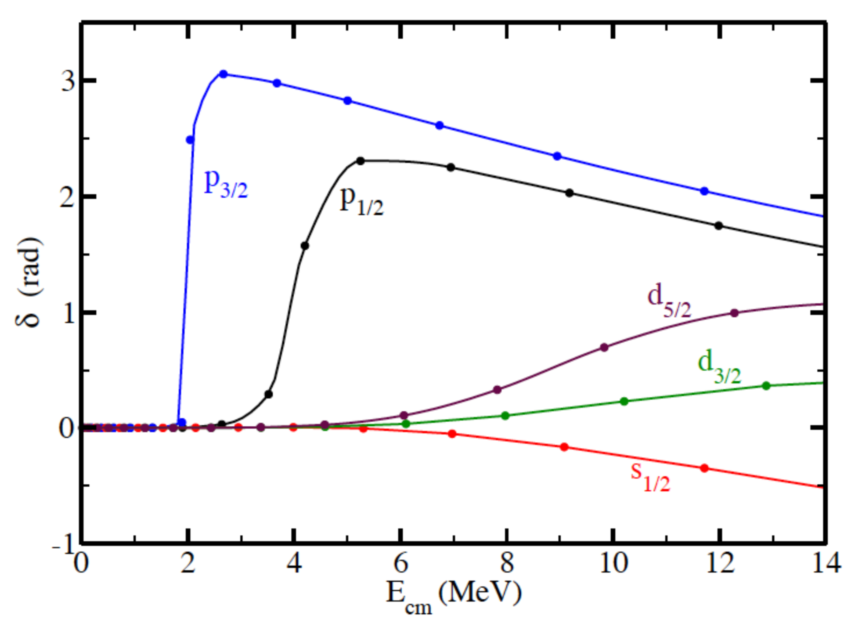
Elastic proton/neutron scattering on 40Ca

The one-nucleon overlap function: $O_A^{A+1}(lj;kr) = \sum_n \left\langle A+1 \left\| \tilde{a}^\dagger_{nlj} \right\| A \right\rangle \phi_{nlj}(r).$

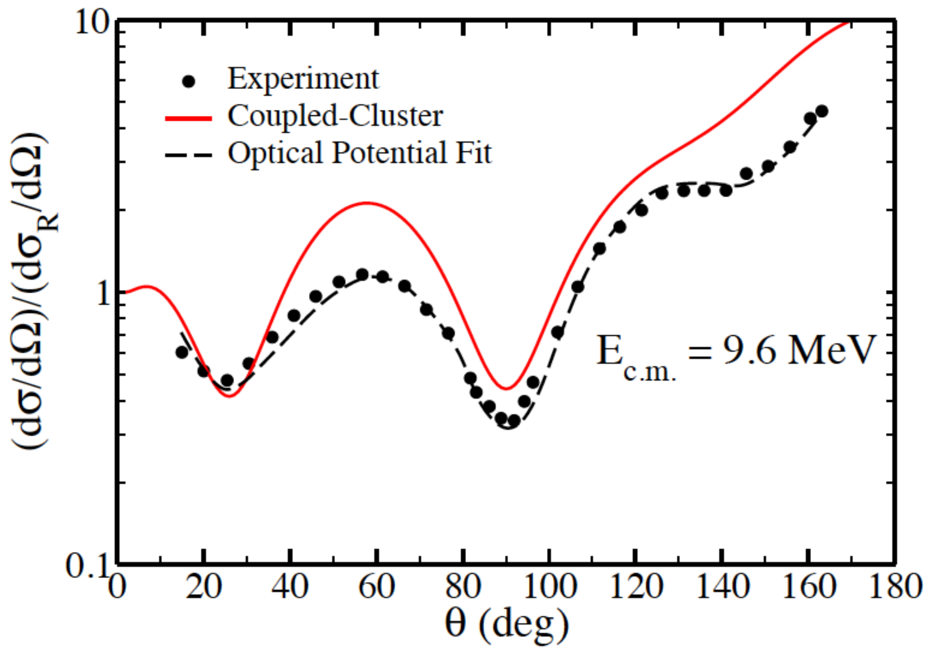
Beyond the range of the nuclear interaction the overlap functions take the form:

$$O_A^{A+1}(lj;kr) = C_{lj} \frac{W_{-\eta,l+1/2}(kr)}{r}, \quad k = i\kappa$$
$$O_A^{A+1}(lj;kr) = C_{lj} \left[F_{\ell,\eta}(kr) - \tan\delta_l(k) G_{\ell,\eta}(kr) \right]$$





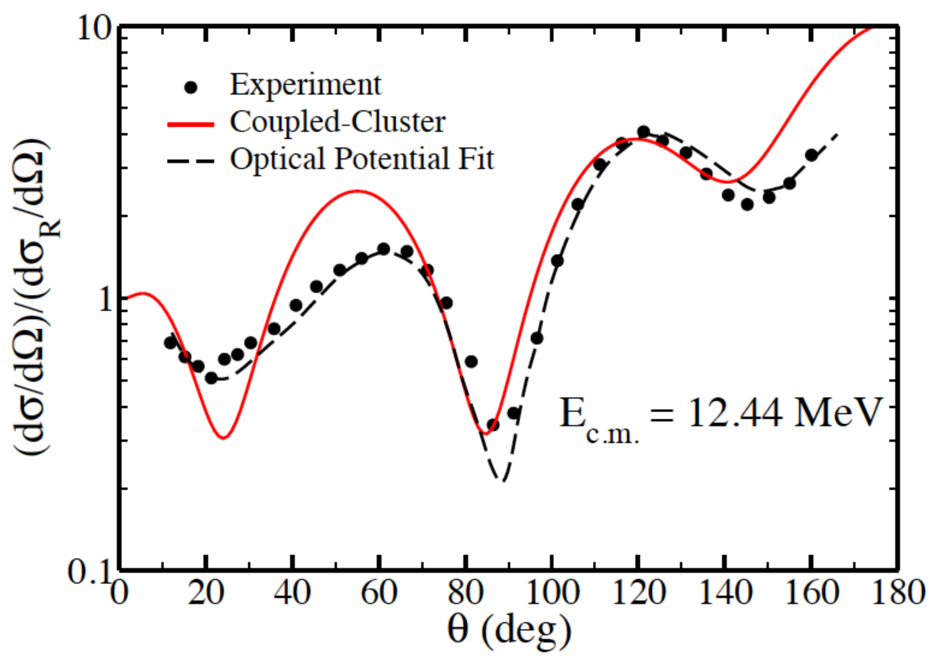
Elastic proton/neutron scattering on 40Ca



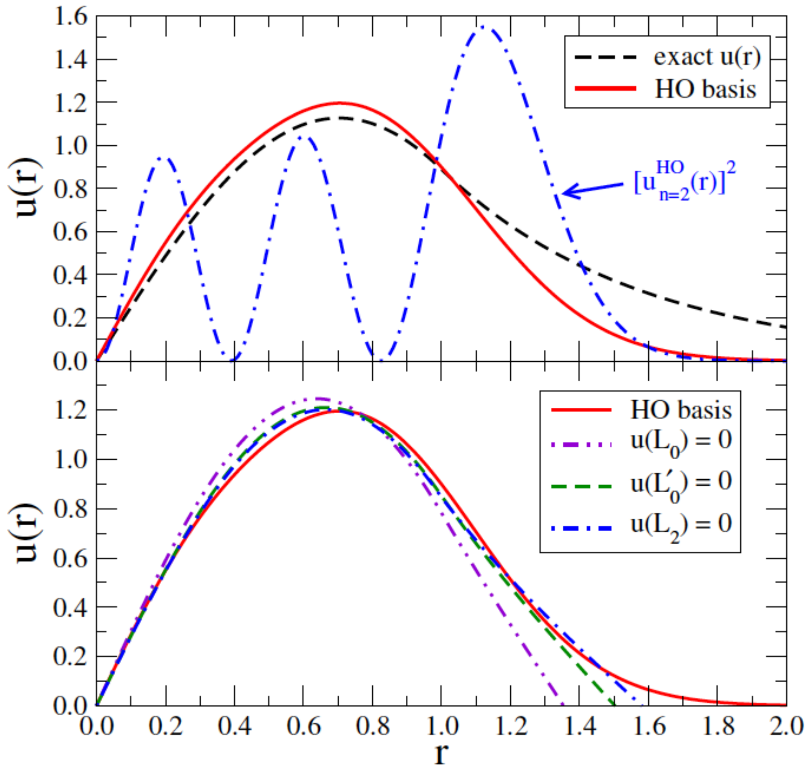
Differential cross section for elastic proton scattering on ^{40}Ca.

Fair agreement between theory and experiment for low-energy scattering.

G. Hagen and N. Michel
Phys. Rev. C **86**, 021602(R) (2012).



What is the infrared cutoff in harmonic oscillator expansions?



Top: Exact wavefunction for a square well potential and the wavefunction from a HO basis expansion with N=4 and hw = 6MeV. Bottom: Wavefunction imposing Dirichlet boundary conditions at L_0, L_0', L_2

For energy/radii extrapolation in a finite HO basis Furnstahl, Hagen, Papenbrock,

PRC 86, 031301 (2012)

A finite Harmonic oscillator basis expansion effectively imposes box boundary conditions at L. Candidates for the infrared cutoff L:

$$L_0 = \sqrt{2(N+3/2)}b$$

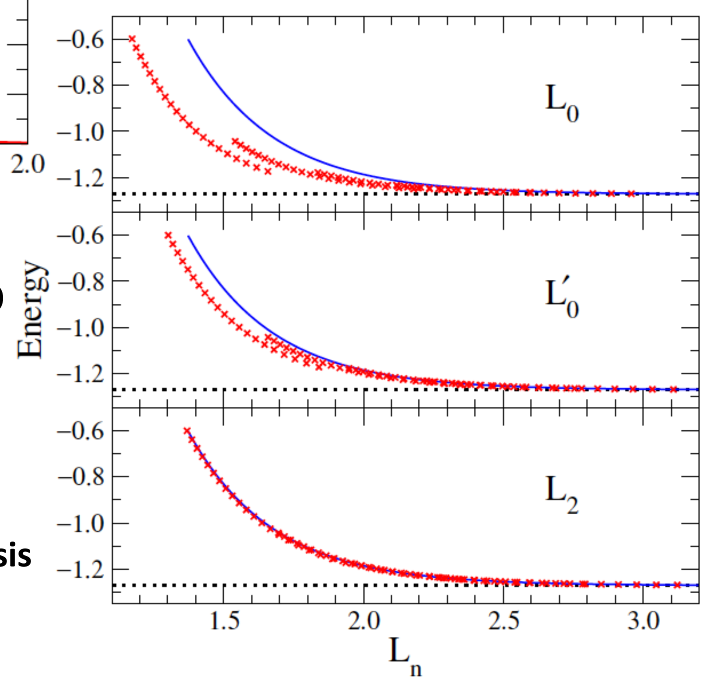
$$L_0' = L_0 + 0.54437b(L_0/b)^{-1/3}$$

$$L_2 = \sqrt{2(N+3/2+2)}b$$

Correct IR cutoff

The energy with Dirichlet boundary conditions at L:

$$E(L) = E_\infty + Ae^{-2k_\infty L} + \mathcal{O}(e^{-4k_\infty L})$$



Solving a two-body problem exactly we can by inspection determine which infrared cutoff is favored.

Clearly L_2 is the right choice!

S. N. More et al, to be published (2013)

Numerical and analytical derivation of L_2

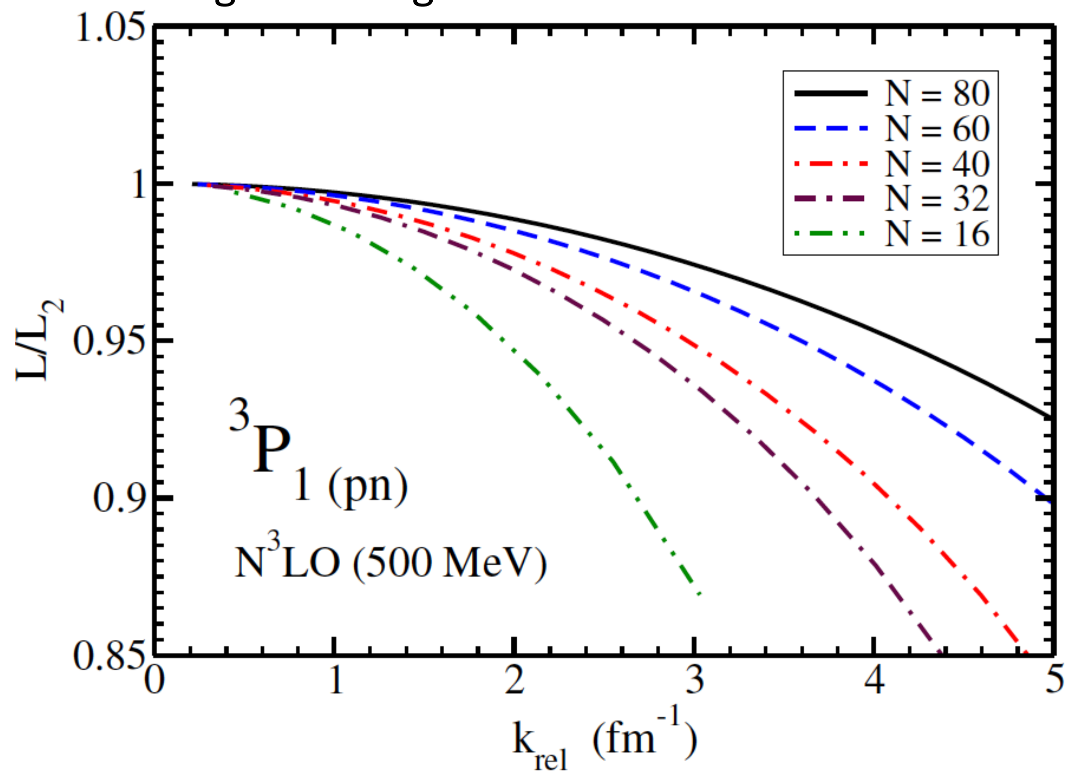
- For s-waves the lowest eigenvalue k_0 of k^2 in a box of size L is π/L
- The lowest eigenvalue of k^2 in a finite HO basis is to a good approximation given by π/L_2
- A finite HO basis imposes a Dirichlet boundary conditions approximately at L_2, it can be shown to be exact for N>>1

N	$\kappa_{\min}$	π/L_2	π/L_0
0	1.2247	1.1874	1.8138
2	0.9586	0.9472	1.1874
4	0.8163	0.8112	0.9472
6	0.7236	0.7207	0.8112
8	0.6568	0.6551	0.7207
10	0.6058	0.6046	0.6551
12	0.5651	0.5642	0.6046
14	0.5316	0.5310	0.5642
16	0.5035	0.5031	0.5310
18	0.4795	0.4791	0.5031
20	0.4585	0.4582	0.4791

We can determine the exact box boundary L for a finite HO basis expansion, by diagonalizing k^2 and for each discrete k_i solve for

$$j_l(k_i L) = 0$$

For increasing HO basis size, the box boundary L approaches L_2 over a large range of energies.



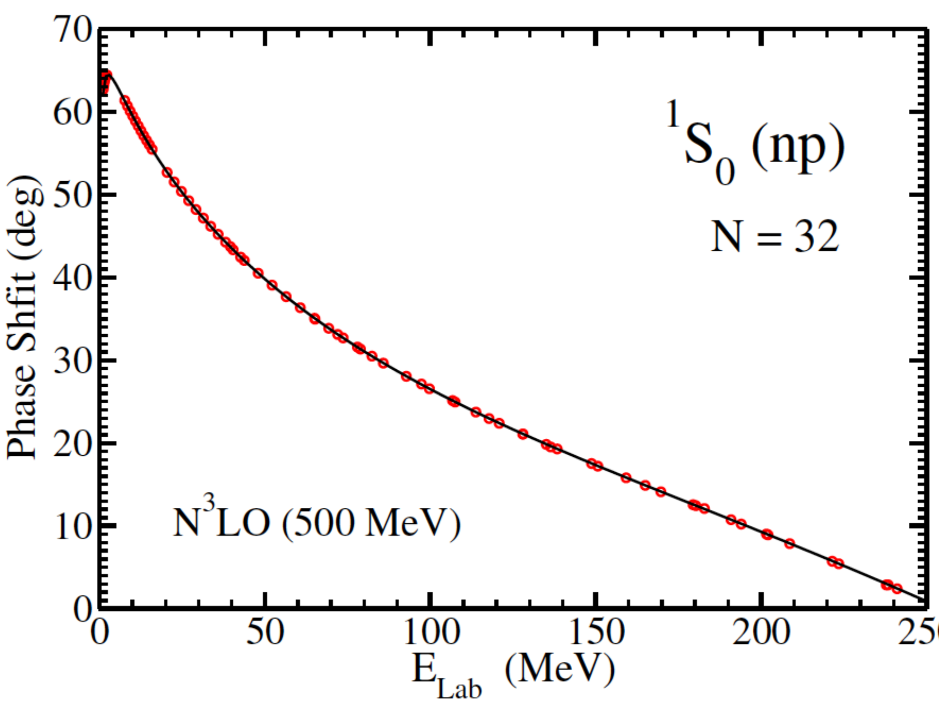
Phaseshifts from a finite Harmonic Oscillator basis

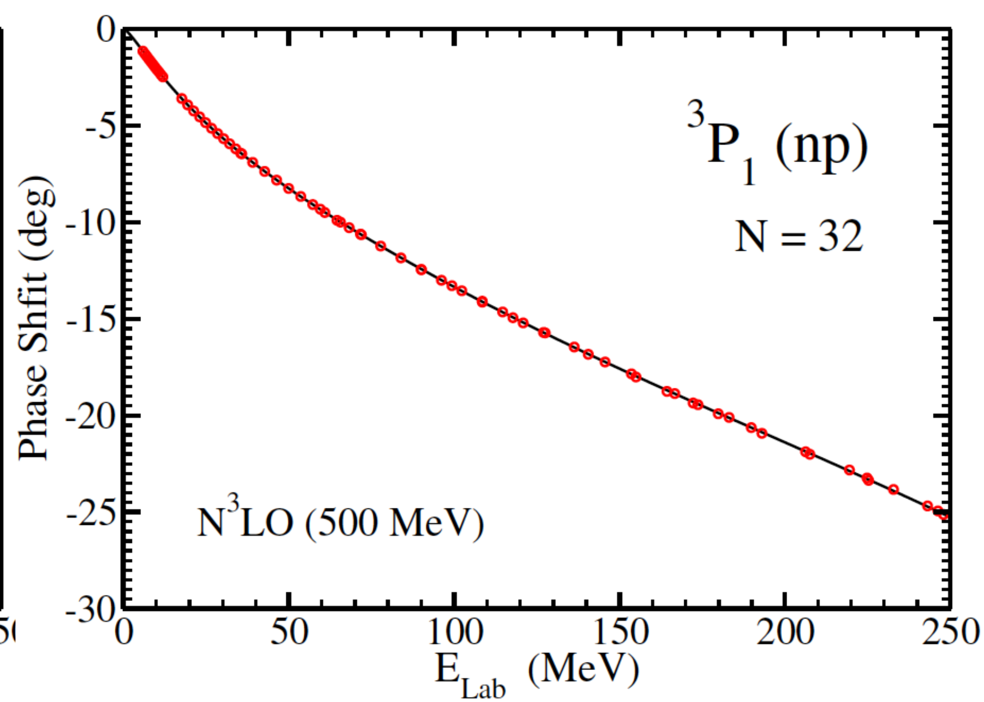
- Diagonalize k^2 in a given finite localized basis such as the Harmonic Oscillator.
- Determine the infrared cutoff or box boundary L as a function of energy by solving the i'th root of

$$j_l(k_i L) = 0$$

- Diagonalize the full Hamiltonian in the given finite basis and obtain the phase shifts from

$$\tan \delta(k_i) = \frac{j_l(k_i L)}{n_l(k_i L)}$$





Summary

1. Interactions from Chiral EFT probed in nuclei
2. CC calculations for oxygen and calcium with effects of 3NF and continuum give significant improvement in binding energy and spectra.
3. Predict weak sub-shell closure in ^{54}Ca.
4. Level ordering in the *gds* shell in neutron calcium is reversed compared to naïve shell model.
5. Predict spin and parity of newly observed resonance peak in ^{24}O.
6. Elastic proton scattering on medium mass nuclei from coupled-cluster theory
7. Phaseshifts from finite harmonic oscillator bases

Treatment of long-range Coulomb effects

We write the Coulomb interaction

$$V_{\rm Coul} = U_{\rm Coul}(r) + [V_{\rm Coul} - U_{\rm Coul}(r)]$$

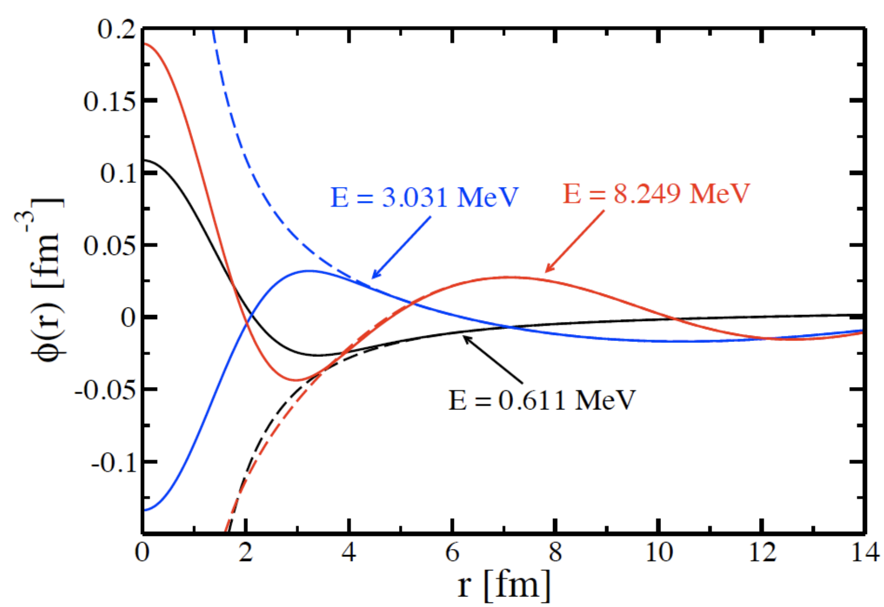
Demanding

$$U_{\rm Coul}(r) \longrightarrow (Z-1)e^2/r \text{ for } r \to +\infty$$

		$s_{1/2}$		$d_{3/2}$		$d_{5/2}$	
N_R	N_T	Re[E]	Γ	Re[E]	Γ	Re[E]	Γ
5	15	1.1054	0.1446	5.0832	1.3519	1.4923	0.0038
5	20	1.1033	0.1483	5.0785	1.3525	1.4873	0.0079
10	25	1.0989	0.1360	5.0765	1.3525	1.4858	0.0093
10	30	1.0986	0.1366	5.0757	1.3529	1.4849	0.0103
15	40	1.0978	0.1351	5.0749	1.3531	1.4842	0.0111
15	50	1.0978	0.1353	5.0746	1.3533	1.4838	0.0114
20	60	1.0976	0.1349	5.0745	1.3533	1.4837	0.0116
30	70	1.0975	0.1346	5.0744	1.3534	1.4837	0.0117
(Michel 2011)		1.0975	0.1346	5.0744	1.3535	1.4836	0.0119

The second term is short range and can be Expanded in Harmonic Oscillator basis. The first term contain the long range Coulomb part:

$$U_{\rm Coul}(k,k') = \langle k| U_{\rm Coul}(r) - \frac{(Z-1)e^2}{r} |k'\rangle + \frac{(Z-1)e^2}{\pi} Q_\ell\left(\frac{k^2+k'^2}{2kk'}\right)$$



We diagonalize the one-body shcrodinger equation in momentum space using the off-diagonal method

N. Michel Phys. Rev. C 83, 034325 (2011)