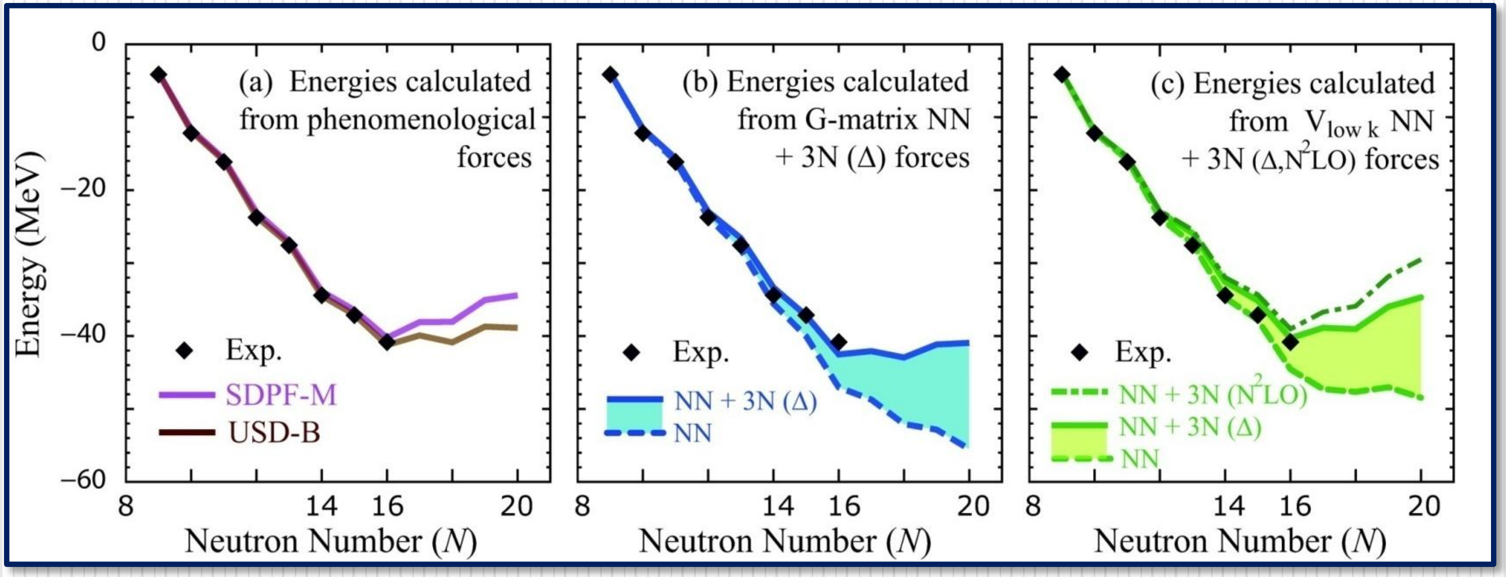
Three-Nucleon Forces for Nuclear Structure in Medium-Mass Nuclei

Jason D. Holt

TRIUMF



INT Program: Effective Field Theory and The Many-Body Problem
May 12, 2009

Outline

- **Microscopic Theory for Valence Shell Effective Interactions**
  - Theoretical method and challenges
  - Deficiencies in method: revealed in monopole part of interaction
- **Interface with Effective Field Theories**
  - NN forces from Chiral EFT evolved to lower momenta
  - 3N forces from Chiral EFT: inclusion in valence-shell interactions
- **Results**
  - Effect on **monopole** part of interaction
  - Applications to nuclear structure in medium mass nuclei
    - Oxygen binding energies and prediction of dripline
    - Ca binding energies and shell gap in ^{48}Ca

Many-body Problem for Finite Nuclei

Various Methods to solve many-body problem: Coupled Cluster, NCSM, In-medium SRG – we use many-body perturbation theory (MBPT)

Solve the many-body Schrödinger equation for nuclear systems:

$H\psi = E\psi$ where $H = H_1 + H_0$ and $H_0 = T + U$ $H_1 = V - U$

- Impossible to solve in heavy systems in complete Hilbert space

-Consider problem in truncated (model) space defined by operators P for model space and Q for excluded space, where

$$P + Q = 1 \quad PQ = 0 \quad PH_{eff}P\psi = EP\psi \quad H_{eff} = H_0 + V_{eff}$$

and V_{eff} acts in the model space given by P

Can obtain "eigenvalue-dependent" H_{eff} (different Hamiltonian for different eigenstates):

$$H_{eff}(E_n) = PHP + PHQ\frac{1}{E_n - QHQ}QHP$$

Folded-diagrams: method to construct eigenvalue-independent effective interaction.

Many-Body Perturbation Theory

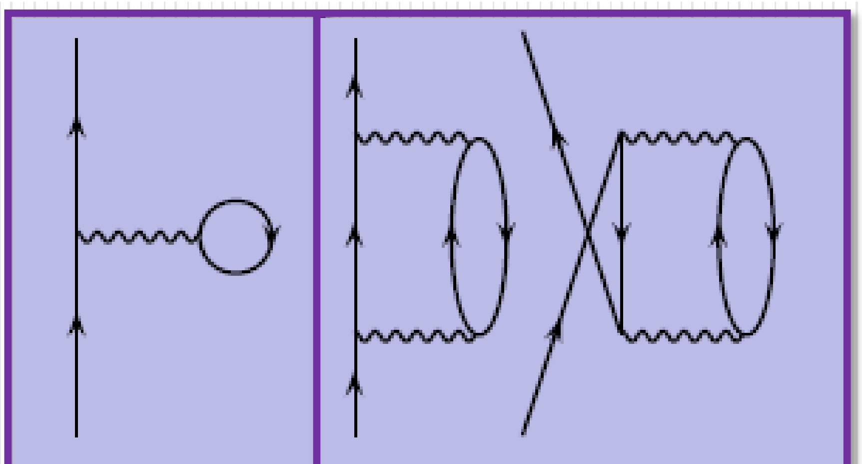
To construct the effective interaction, introduce:

$$\hat{Q}(\omega) = PH_1P + PH_1Q\frac{1}{\omega - QHQ}QH_1P$$

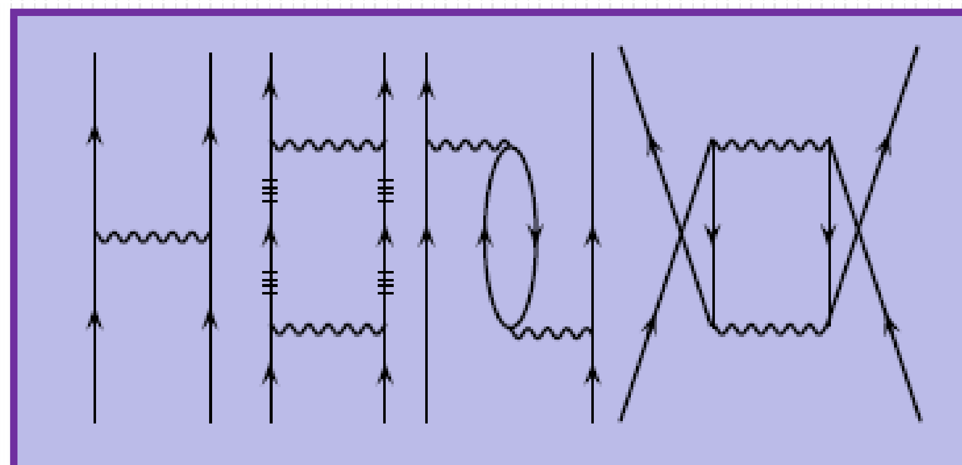
$\hat{Q}(\omega)$-box: sum of all possible topologically distinct diagrams which are:

- **Irreducible:** the intermediate many-particle states between each pair of vertices belong to the Q space.

- **Valence linked**: all the interaction vertices are linked (via fermion lines) to at least one valence space line.



1-body Q-box to 2nd order



2-body Q-box to 2nd order

Effective Interaction

Effective interaction given by infinite series of “folded” diagrams:

$$V_{\rm eff} = \hat{Q} - \hat{Q}' \int \hat{Q} + \hat{Q}' \int \hat{Q} \int \hat{Q} - \hat{Q}' \int \hat{Q} \int \hat{Q} \int \hat{Q} + \dots$$

$\int$ = generalized folding operator – removes divergences due to degenerate model space

Several ways to solve the infinite series

Assuming degenerate model space, $PH_0P = \omega P$, can obtain V_{eff} from Lee-Suzuki iterative scheme:

$$V_{eff}^{(n)} = \left(1 - Q_1 - \sum_{m=2}^{n-1} \hat{Q}_m \prod_{k=n-m+1}^{n-1} V_{eff}^{(k)}\right)^{-1} \hat{Q}(\omega_0) \qquad \hat{Q}_m = \frac{1}{m!} \frac{d^m \hat{Q}(\omega)}{d\omega^m}$$

Need to determine 1- and 2-body Q-box and its derivatives

Details of Calculation

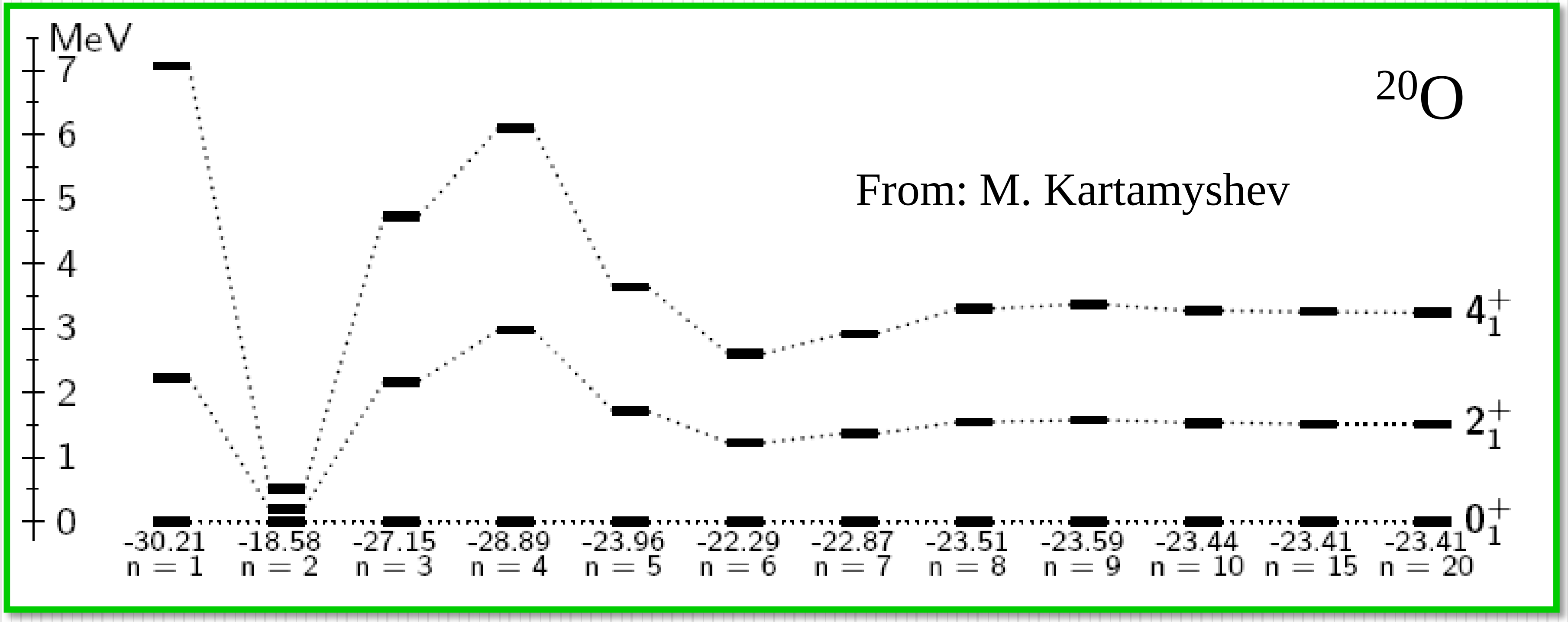
Assume degenerate model space

Intermediate states excitations: 6 major shells above model space

Neglect 3-body and higher Q-box

LS iterative scheme: converged ~10 iterations

2nd-order in Perturbation Theory



Monopole Part of Interaction

Microscopic MBPT typically works for few particles/holes away from closed shell: deteriorates beyond this

- Deficiencies in microscopic interactions can be improved by adjusting monopole two body matrix elements:

Angular average of interaction

Determines interaction of orbit *a* with *b*

$$V_{ab}^{T} = \frac{\sum_J (2J+1) V_{abab}^{JT} [1-(-1)^{J+T}\delta_{ab}]}{\sum_J (2J+1)[1-(-1)^{J+T}\delta_{ab}]}$$

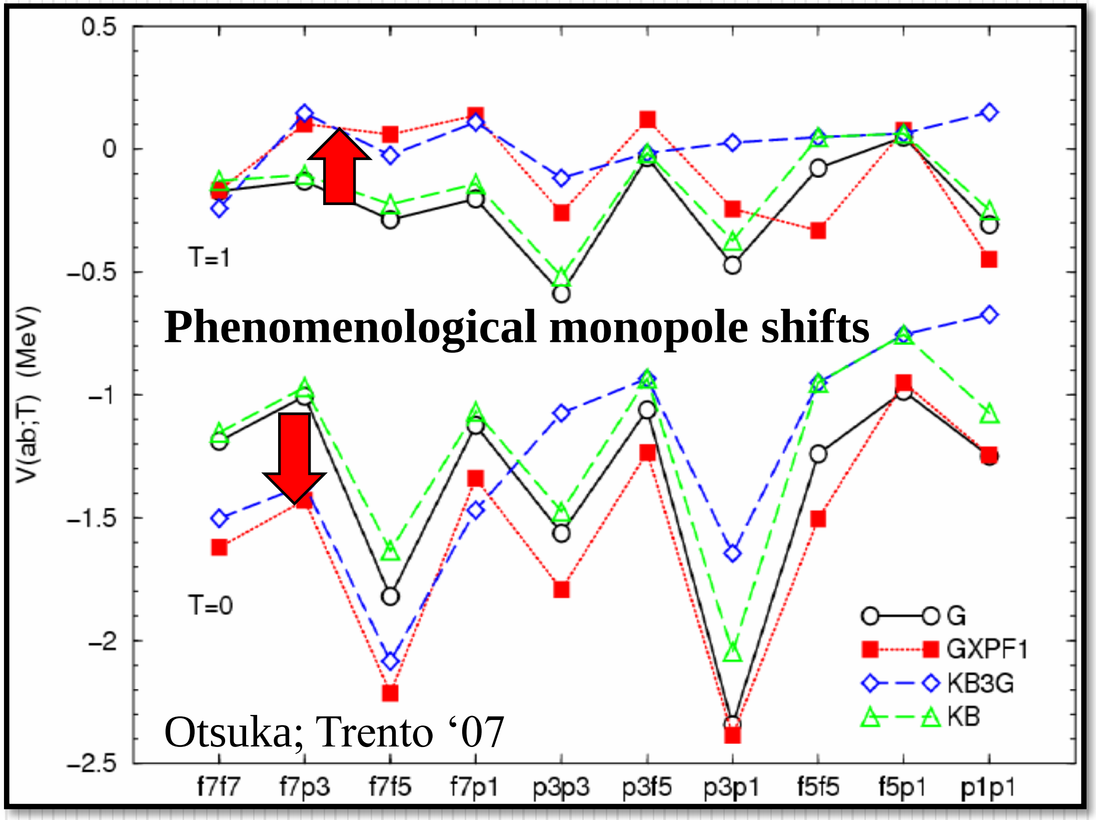
Phenomenological shell model interactions typically start from MBPT results then exploit importance of monopoles:

sd-shell: USD (1984), USDa, USDb (2006)
- global fit of SPE and TBME; monopoles most important

pf-shell:
- GXPF1 (2004): quasi-global fit; monopoles most important
- KB3G(2001): modification of monopole part only

Monopole Hamiltonian determines evolution of SPEs
- important for determining shell closures

Phenomenological vs. Microscopic



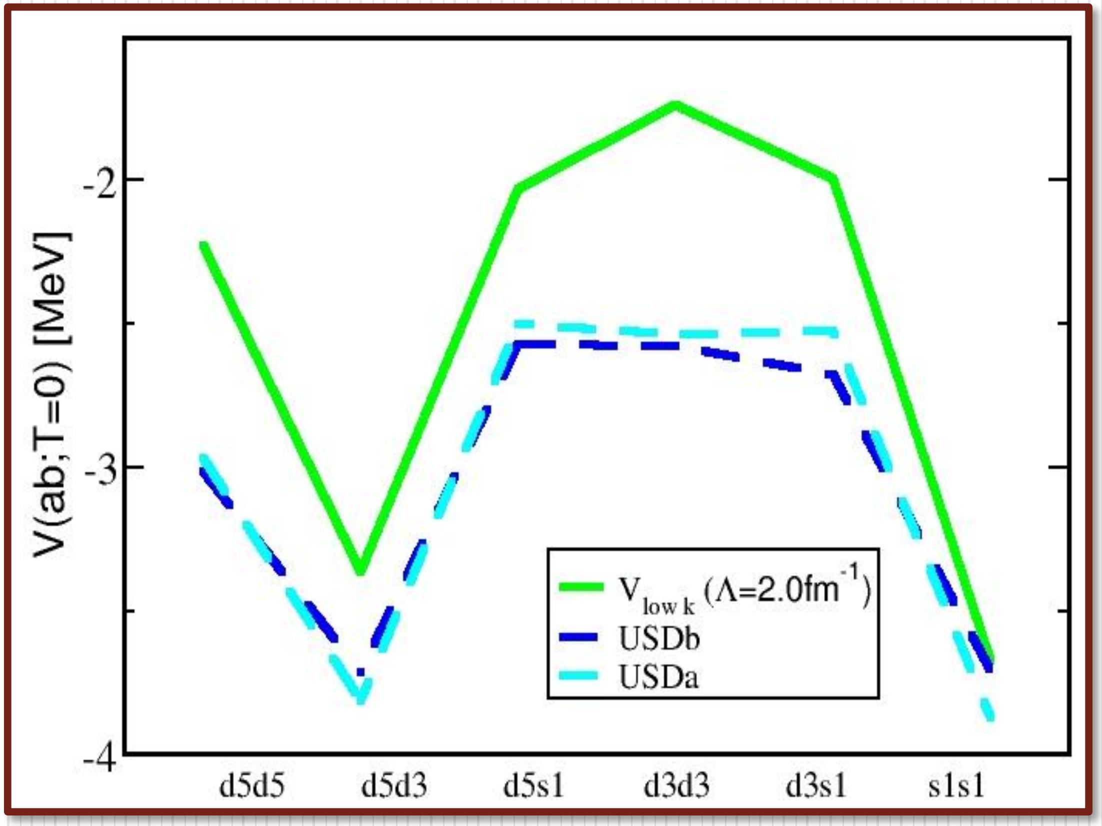
Compare monopoles from:

- *Microscopic* **G-matrix**, **Kuo-Brown** interactions
- *Phenomenological* **GXPF1**, **KB3G** interactions.

Clear shifts for low-lying orbitals:

- T=1 repulsive shift
- T=0 attractive shift

Phenomenological vs. Microscopic



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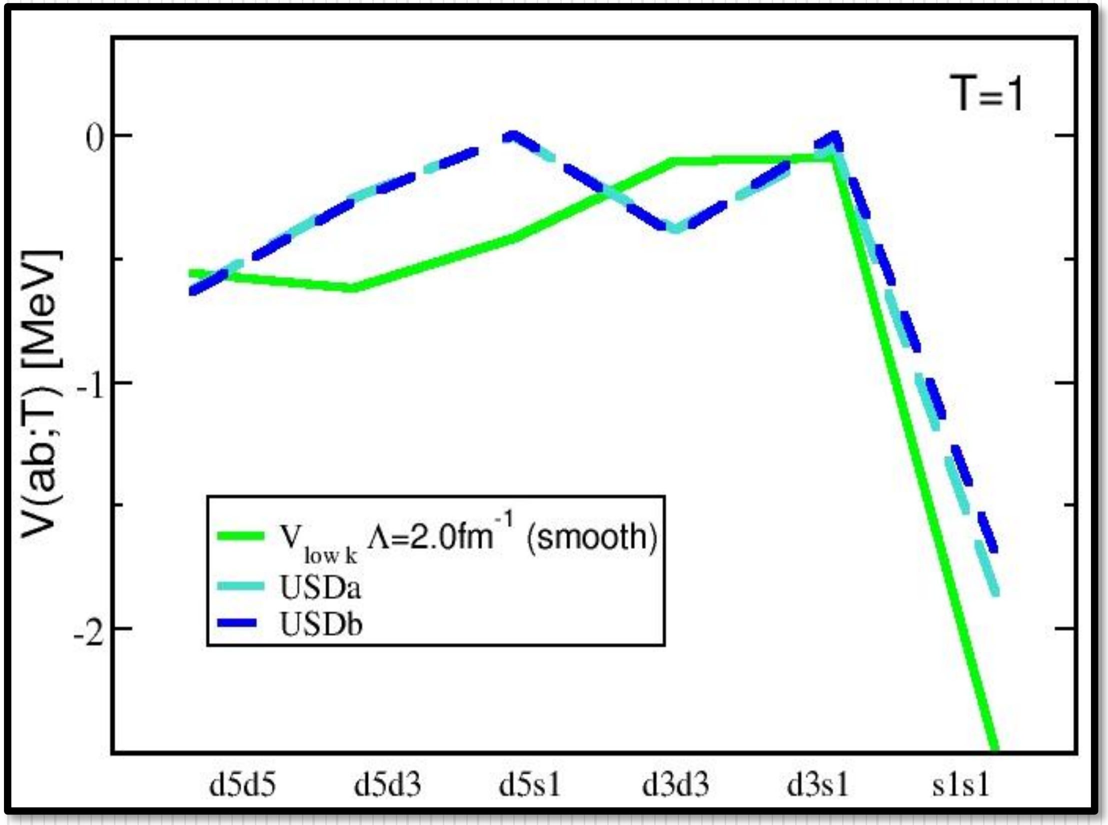
Similar for sd-shell: USDa,USDb interactions: T=0 attractive

Phenomenological vs. Microscopic



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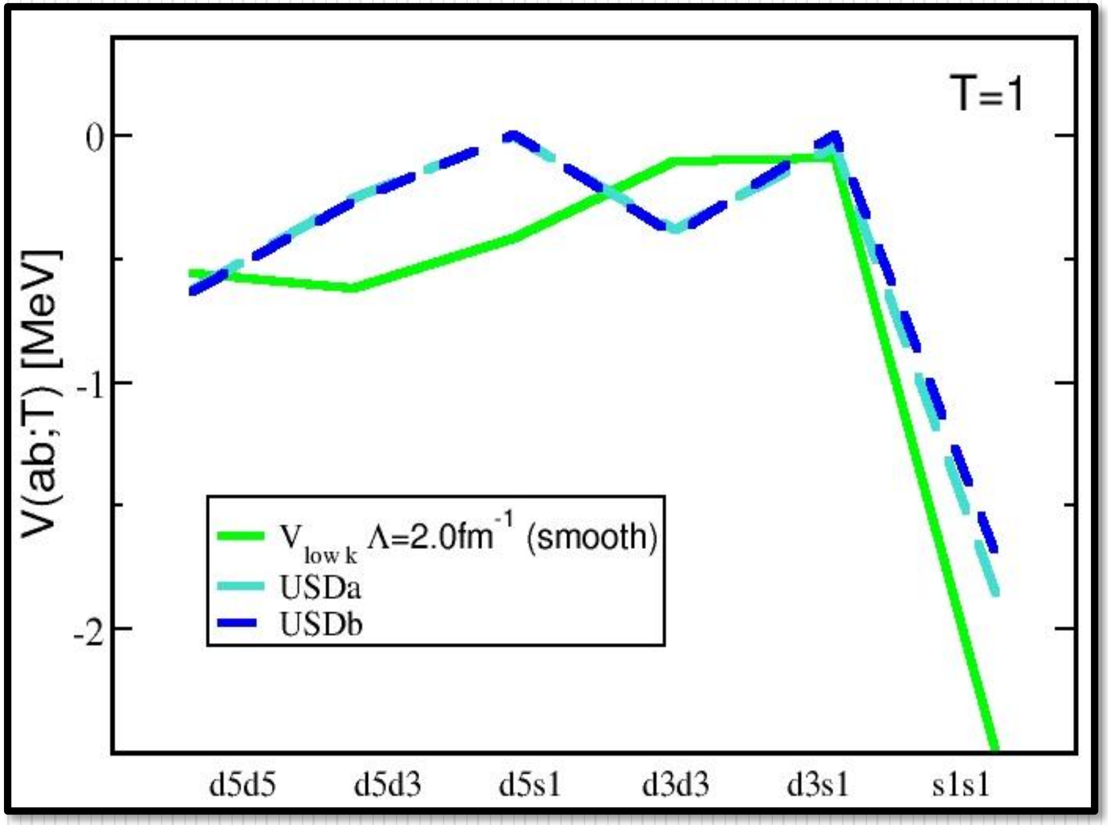

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Cause of the shifts?

MBPT converged? Investigating 3rd order diagrams in Q-box

In Progress: Validate against No-Core Shell Model with a core

with: B. Barrett, A. Lisetskiy, and A. Schwenk

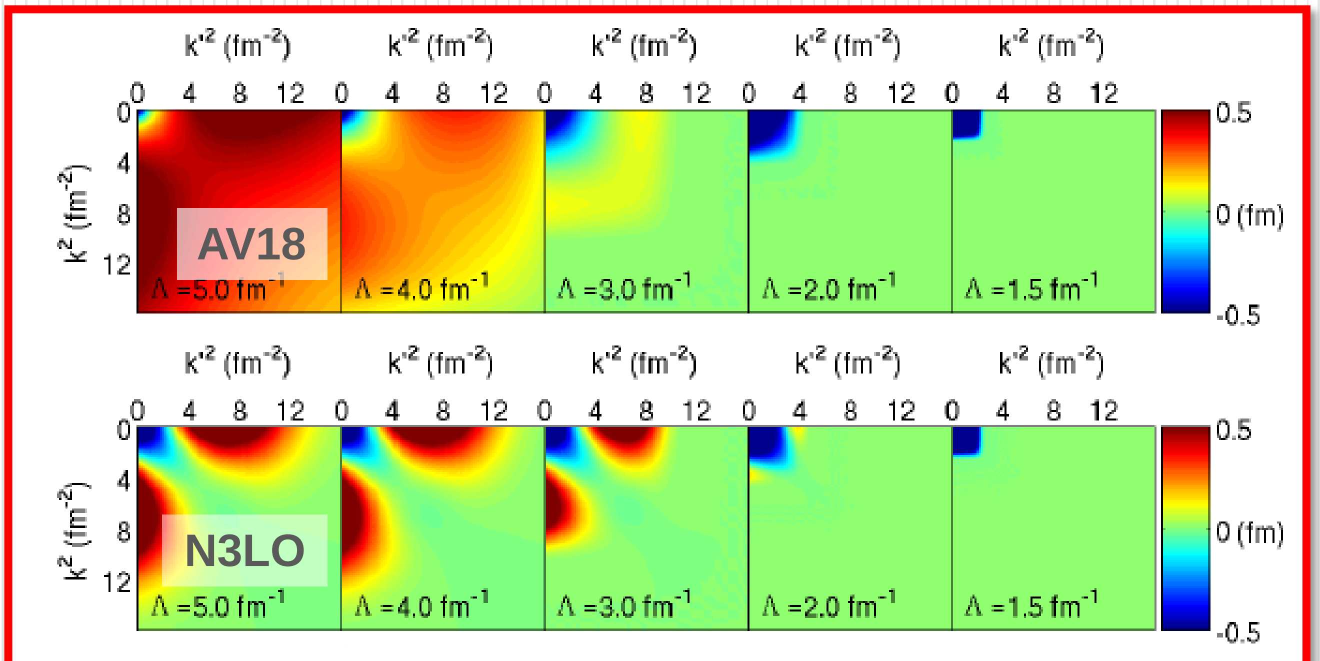
Can 3N forces explain these shifts? -- Zuker (2003)

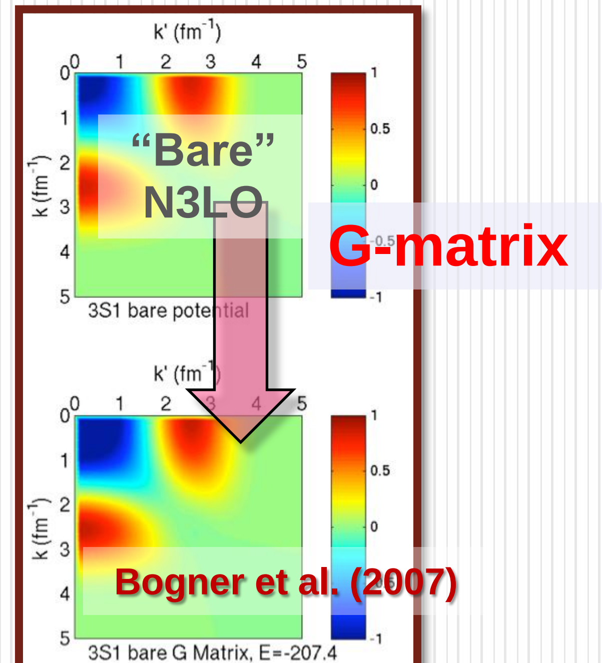
Nuclear Interactions

$$H(\Lambda) = T + V_{\rm NN}(\Lambda) + V_{\rm 3N}(\Lambda) + V_{\rm 4N}(\Lambda) + \ldots$$

Chiral interactions provide systematic, consistent 3N

Chiral 2N: large cutoffs not suitable for MBPT – need to renormalize
    Evolve to lower cutoff using RG methods (smooth regulator)





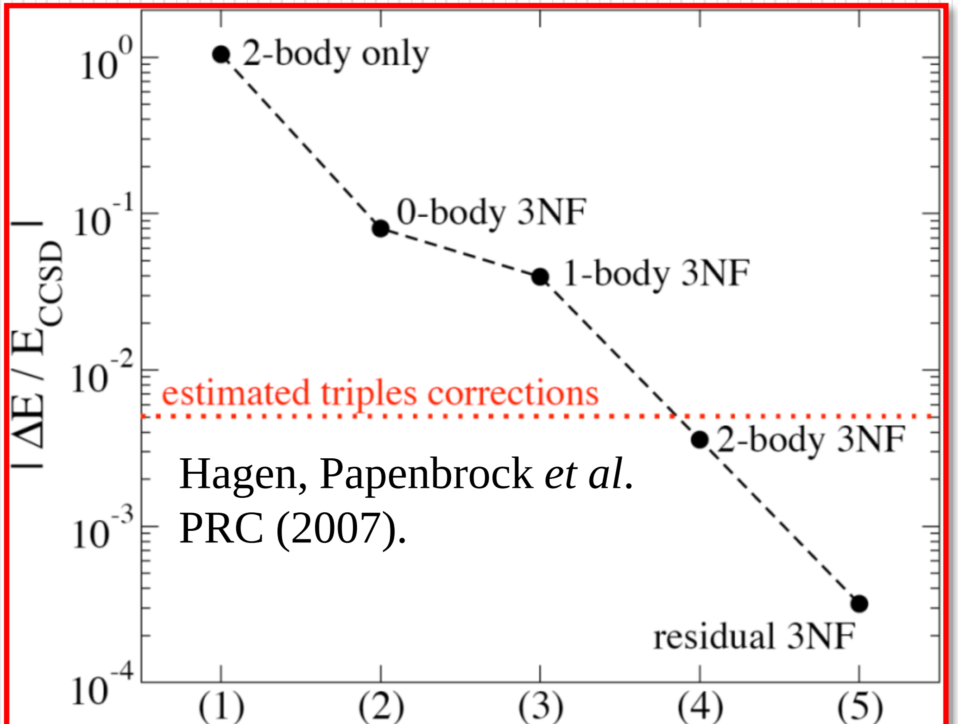
Lower cutoffs: improve convergence for structure in light nuclei, perturbative in nuclear matter – off-diagonal couplings removed (remain for G-matrix)

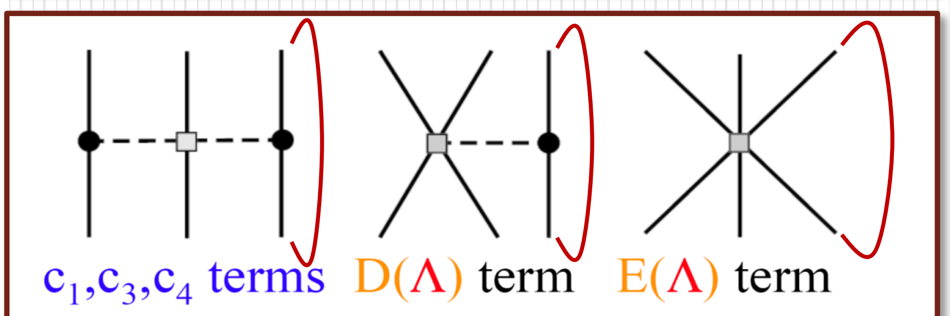
3N Forces in Valence-Shell Interactions

$V_{\text{low }k}(\Lambda)$ + leading order chiral $V_{3N}(\Lambda)$

$D(\Lambda)$, $E(\Lambda)$ couplings fit to ^{3}H BE, ^{4}He radius for given Λ

Approach: inspired by **Coupled Cluster** results for ^{4}He





Benchmarked using low-momentum Interactions and 3NF

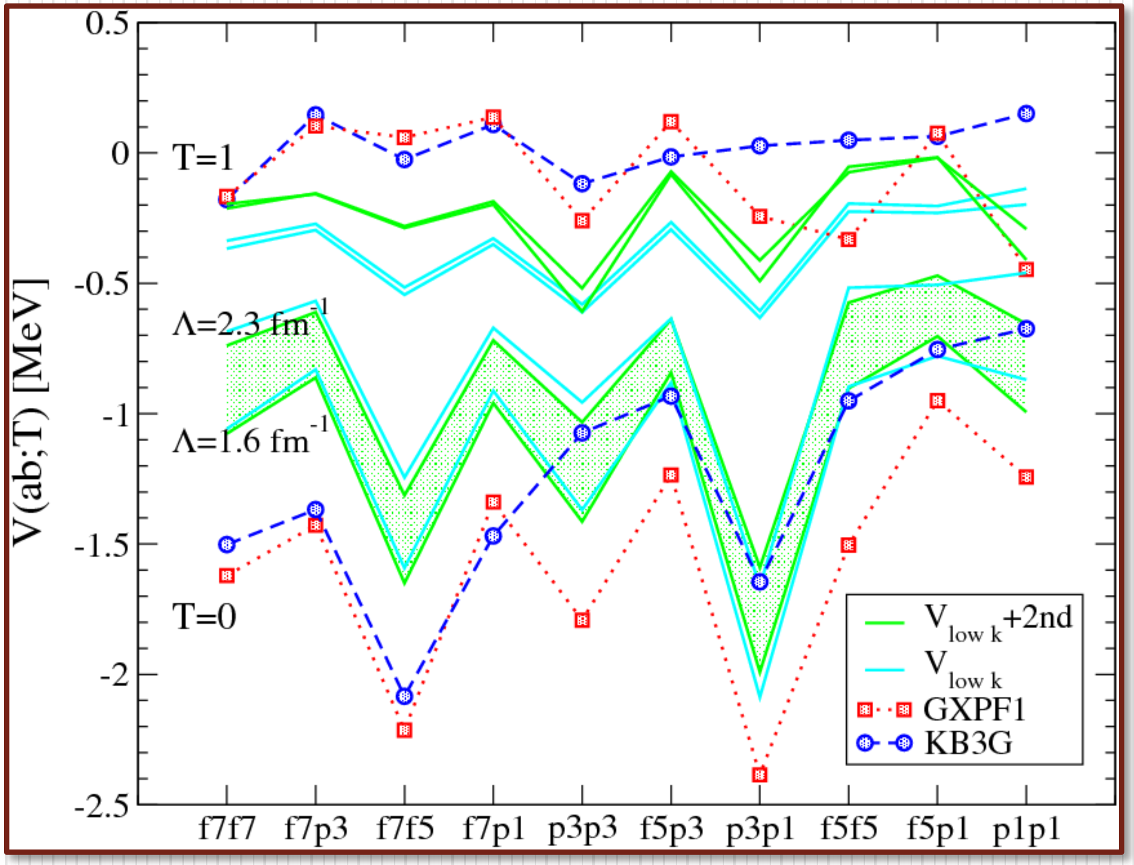
- 0- 1- and 2-body parts of 3NF dominate – **neglect residual 3NF**
- Sum over occupied states (as in coupled cluster, nuclear matter):

$$\langle ab | V_{3N,\text{eff}} | a'b' \rangle = \sum_{c=core} \langle abc | V_{3N} | a'b'c \rangle$$

- 3N forces tractable in shell model

Cutoff Dependence of Monopoles

Use cutoff dependence of $V_{\text{low }k}(\Lambda)$ to probe effects of 3N force:



T=1: cutoff-independent monopoles

- Indicates **c** terms may dominate (repulsive contribution in nuclear matter)

T=0: large cutoff dependence

- Expect attraction from 2nd order NN-3N

- Not enough to calculate effects to first order only for T=0

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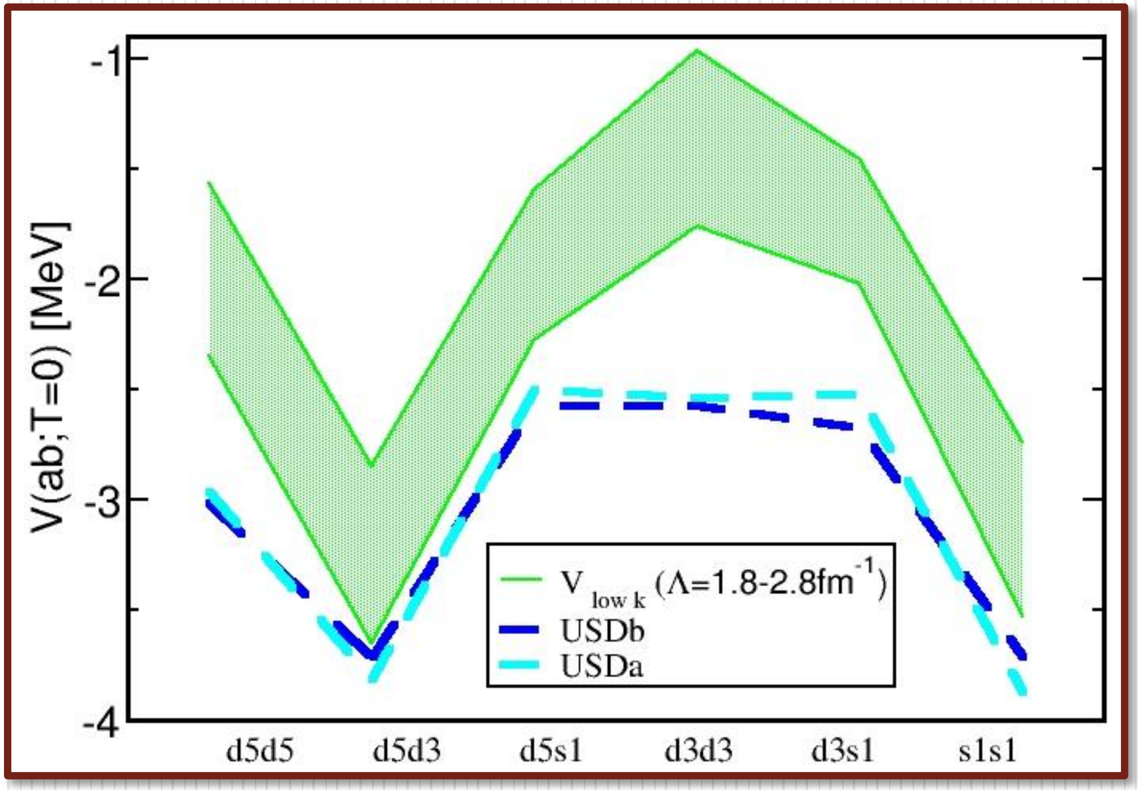

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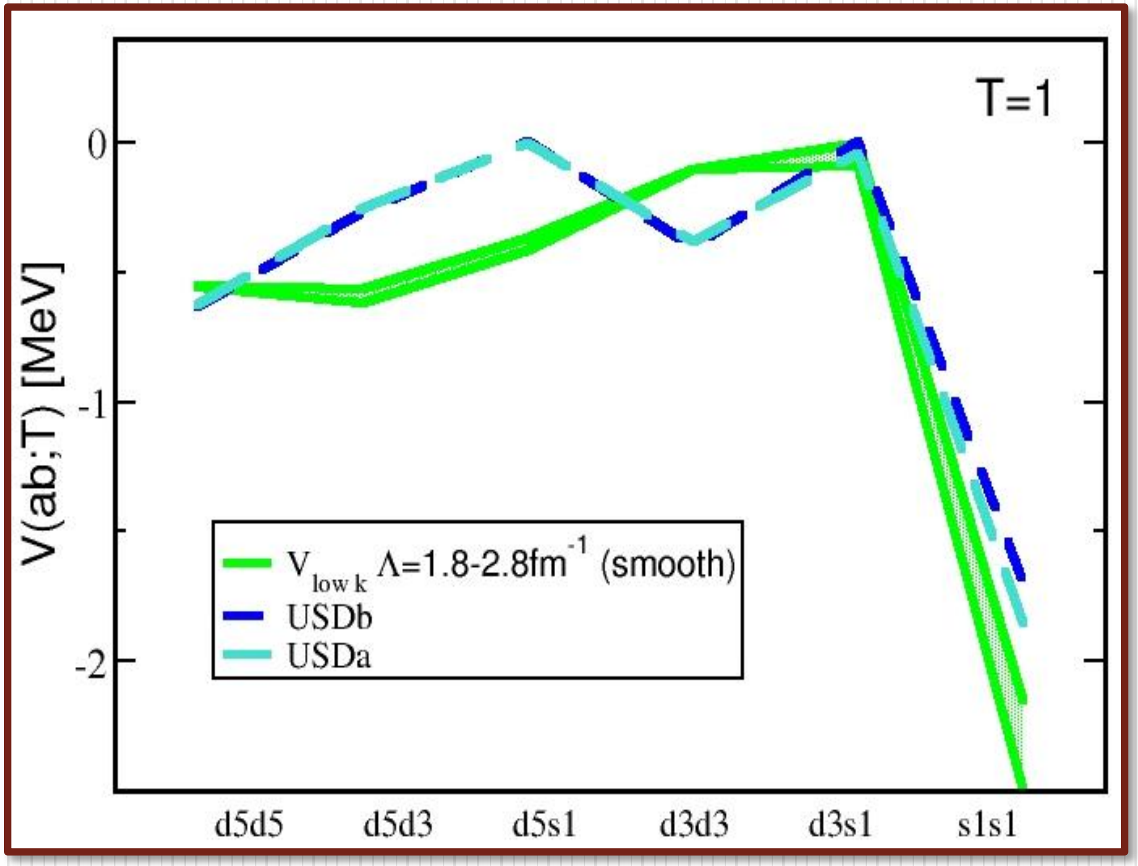


T=1: cutoff-independent monopoles

- Indicates **c** terms may dominate (repulsive contribution in nuclear matter)

T=0: large cutoff dependence

- Expect attraction from 2nd order NN-3N

- Similar trends in sd-shell
- Wrong hierarchy for low-lying T=1 monopoles with microscopic theory

Calculation Scenarios

Focus on T=1 monopoles and systems in the following scenarios:

1 NN matrix elements derived from:

- Chiral N^3LO (500MeV) using smooth-regulator $V_{low\ k}$ with range of cutoffs

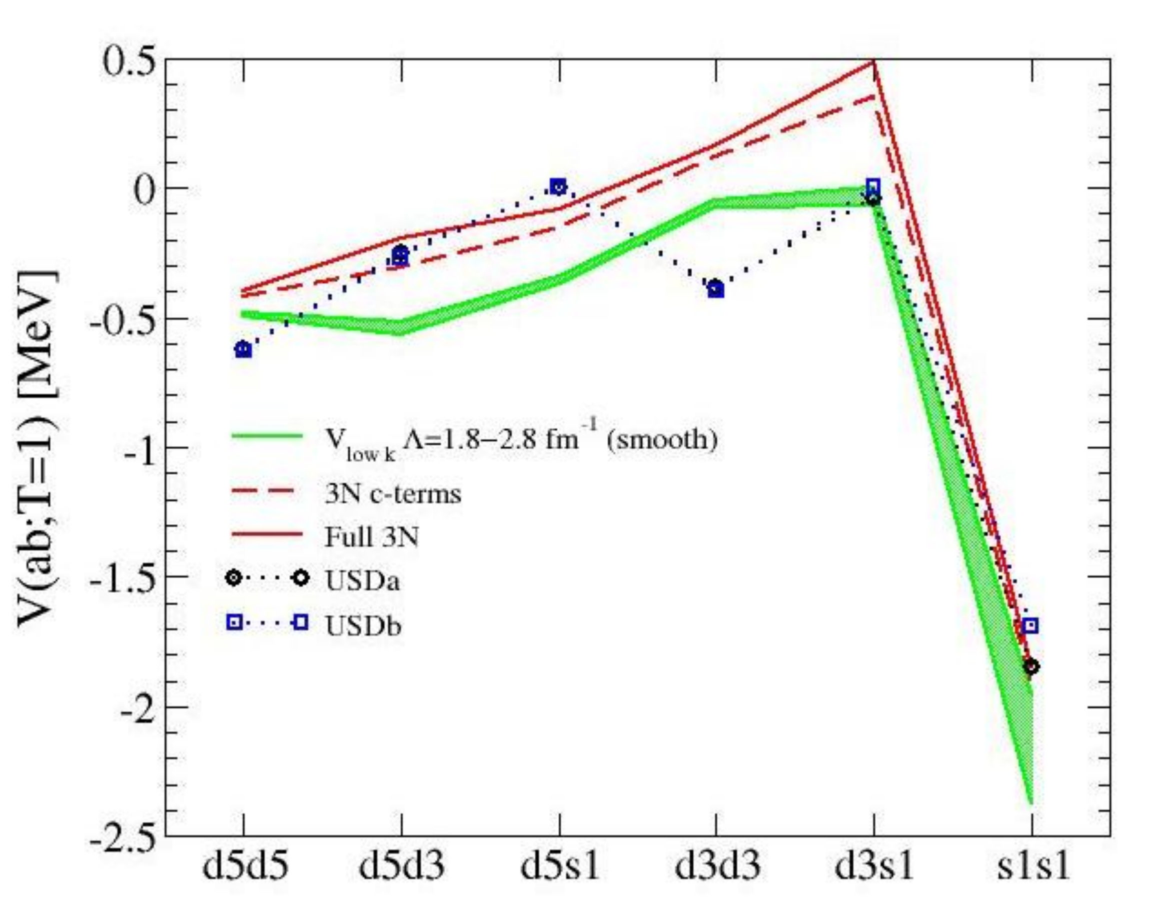
- 2^{nd} order in MBPT: details as previously given

2 Monopoles derived from 3N Forces

A) One-Delta excitation from N^2LO: $c_1 = 0, c_3 = -2c_4 = \frac{h_A^2}{9\Delta m}; h_A = \frac{3g_A}{\sqrt{2}}$

B) Full Chiral N^2LO

T=1 Monopoles in *sd*-shell



- 3N calculated to first order in MBPT
- Converged in 3NF partial waves up to: $J \le \frac{7}{2}$

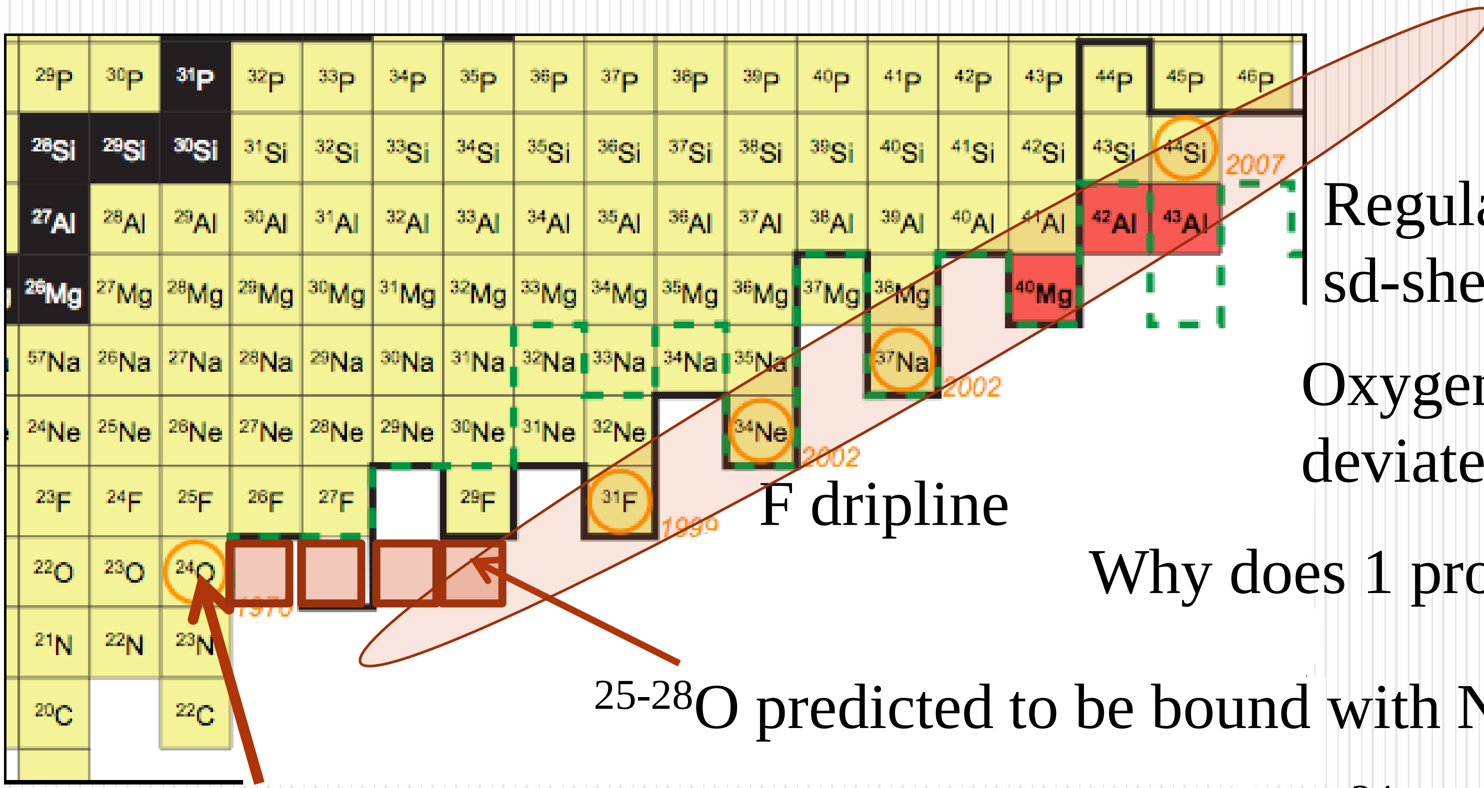
3N (one-Δ)

3N (full N²LO)

- Dominant effect from **one-Δ** – as expected from cutoff variation

- 3N forces produce clear repulsive shift in monopoles
- Restores monopole hierarchy $d_{5/2}$-$d_{5/2}$ vs. $d_{5/2}$-$d_{3/2}$
- Improved treatment of $d_{3/2}$ – treat as holes in ^{40}Ca core

Oxygen-Flourine Anomaly



Regular trend for dripline of sd-shell nuclei

Oxygen dripline observed to deviate from this trend

F dripline

Why does 1 proton change so much?

$^{25-28}$O predicted to be bound with NN-only

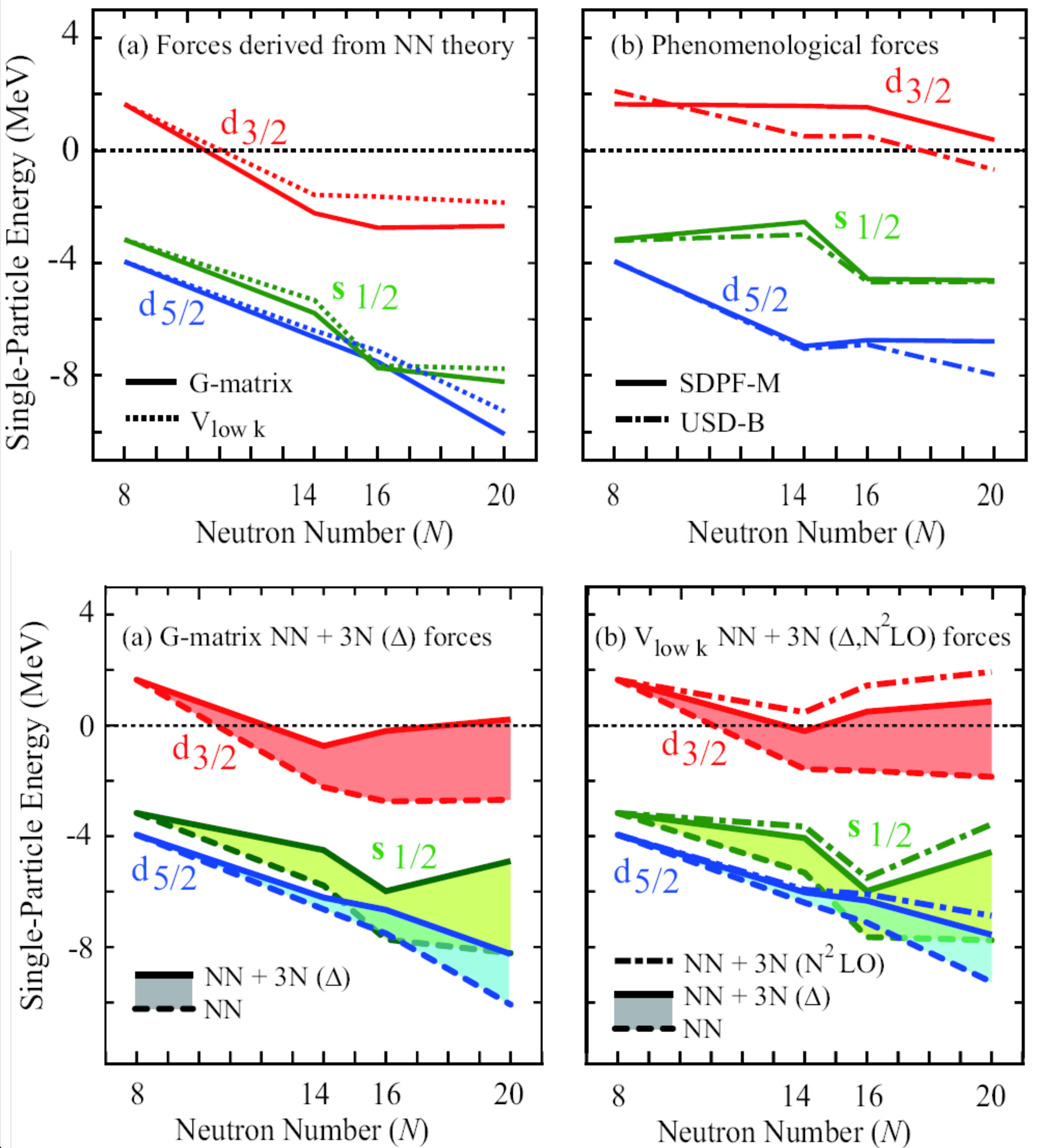
Experimental Oxygen dripline observed at ^{24}O

Monopole changes multiplied by neutron number – small changes will impact neutron-rich regions

Use 3N forces to investigate this anomaly – probe limits of nuclear existence with microscopic theory

Evolution of SPEs in sd-shell

First results with 3N forces



$d_{3/2}$ orbit bound for microscopic NN-only interactions (G-matrix and $V_{low\ k}$)

NN predicts bound Oxygen isotopes to ^{28}O

Additional repulsion in $d_{3/2}$ monopole strengths from 3N multiplied by neutron number

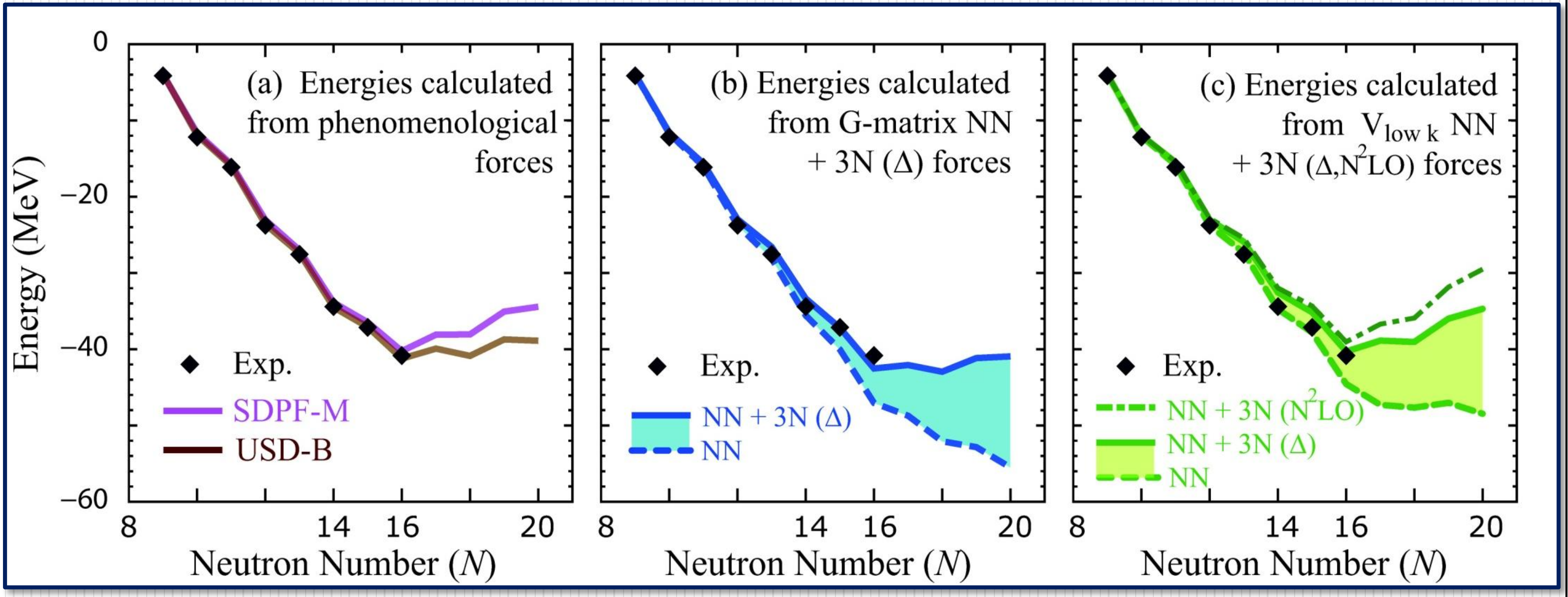
Largest effect seen in neutron rich isotopes

$d_{3/2}$ becomes unbound orbit with addition of 3N forces

Similar behavior for single Δ and chiral N^{2}LO forces

Calculated Oxygen Binding Energies

- First shell-model calculations using NN+3N monopoles: predict dripline in O
- Calculate GS energies (relative to ^{16}O) with SDPF-M single particle energies using MBPT to 2nd order, 6 major shell intermediate state excitations



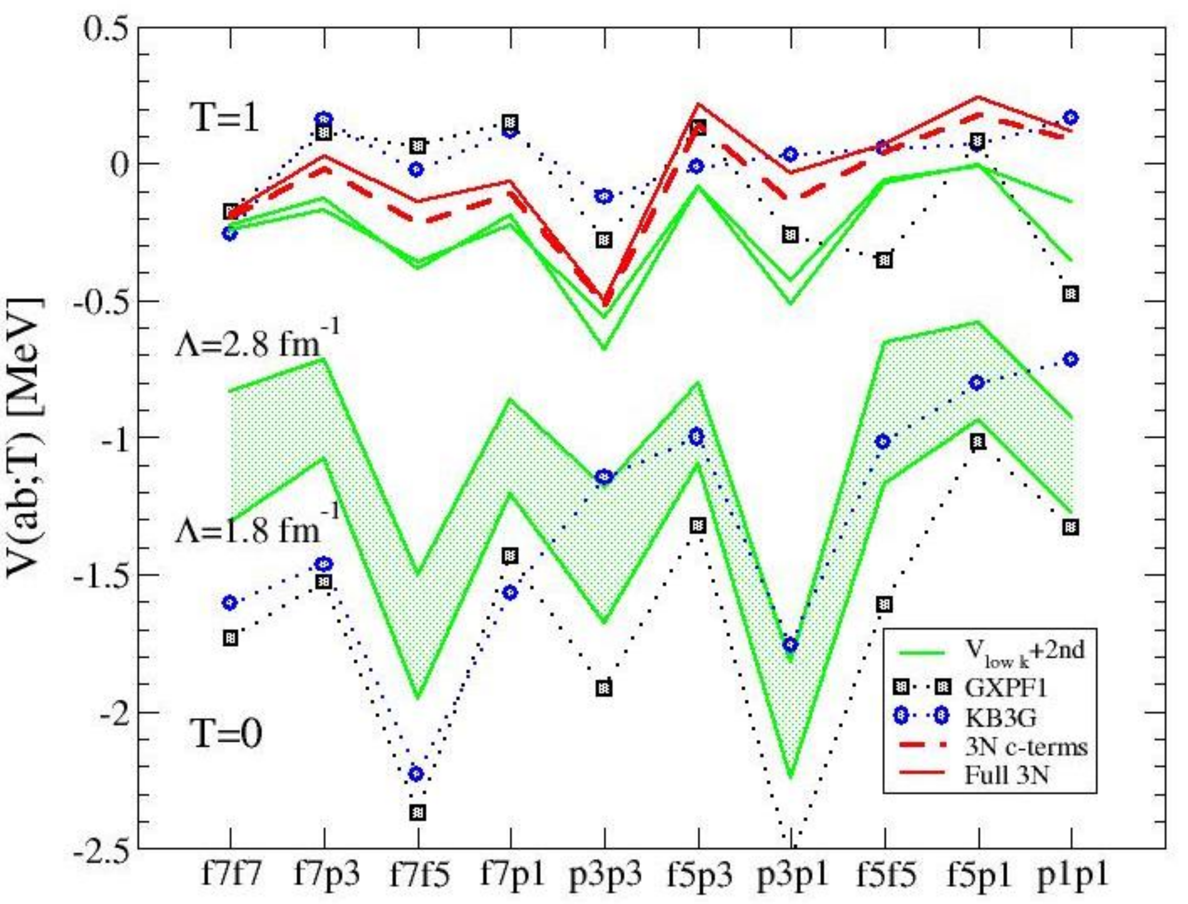
Phenomenological interactions show $^{25-28}O$ less bound than ^{24}O

BEs increase for NN-only through ^{28}O

Adding 3NF: isotopes beyond ^{24}O less bound: dripline correctly predicted at ^{24}O!

Monopoles in *pf*-shell

- Similar picture as in sd-shell



- Calculated to first order in many-body perturbation theory
- converged with 3NF partial waves up to: $J \leq \frac{7}{2}$

  3N (one Δ)

  3N (N^2LO)

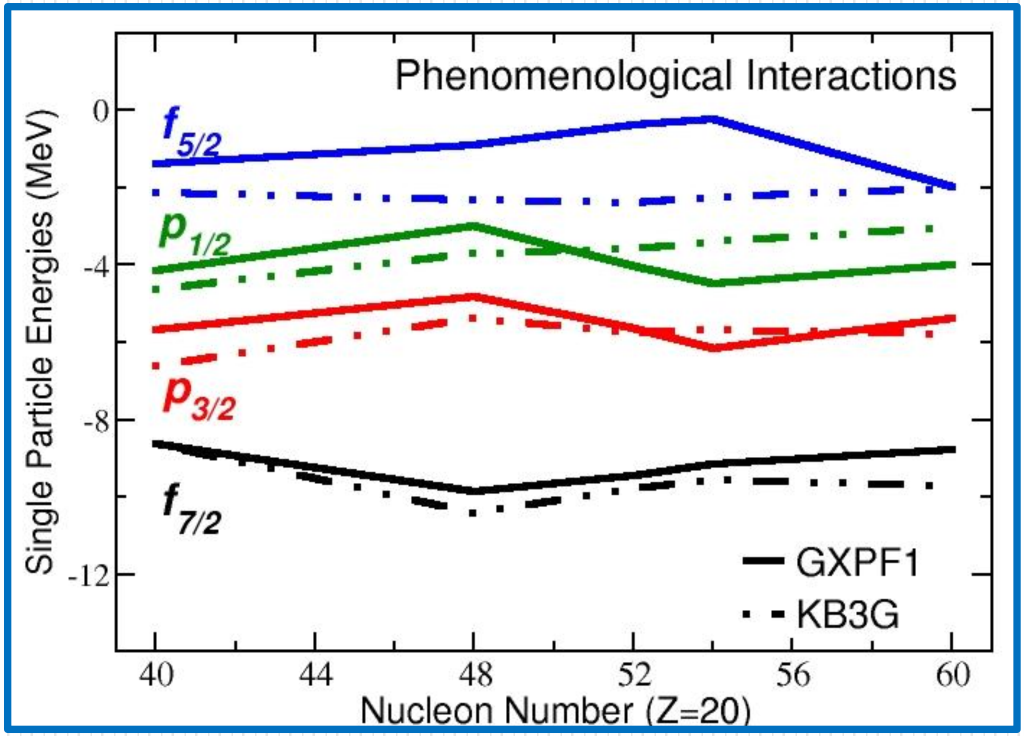
- Clear repulsive shift due to 3NF in T=1 channel

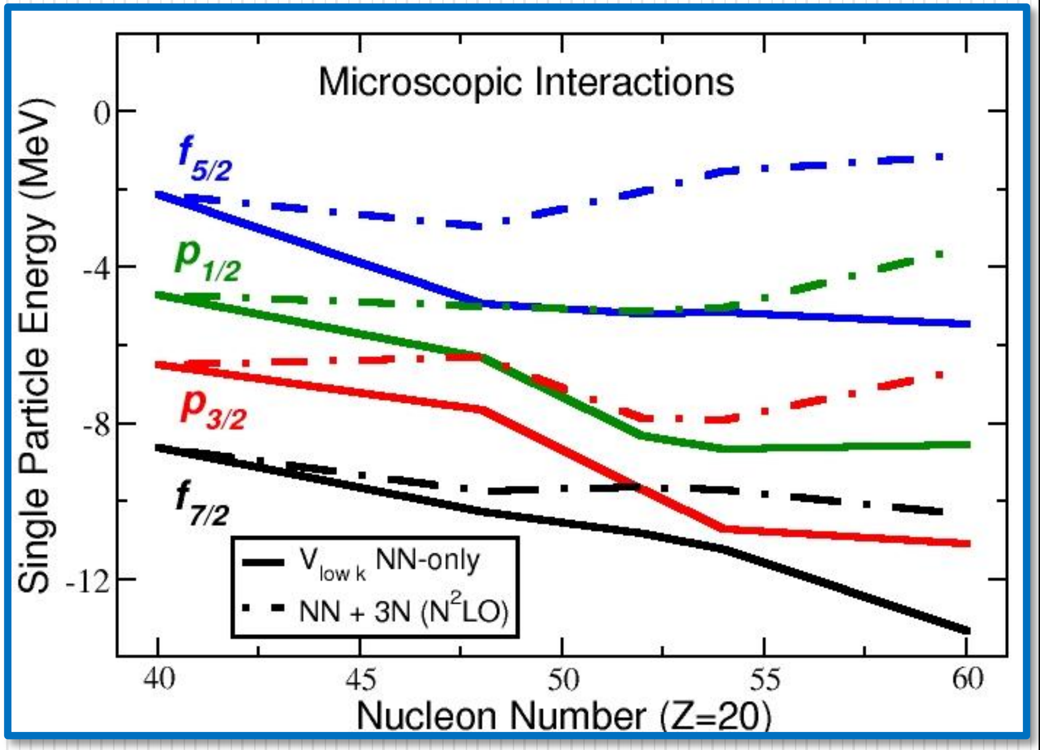
T=0: Expect attraction from 2nd order perturbation theory: **in progress**

Calcium Effective Single Particle Energies

Using KB3G SPEs, MBPT with 3 major shells (preliminary)

Calculate SPEs with 3N force monopoles





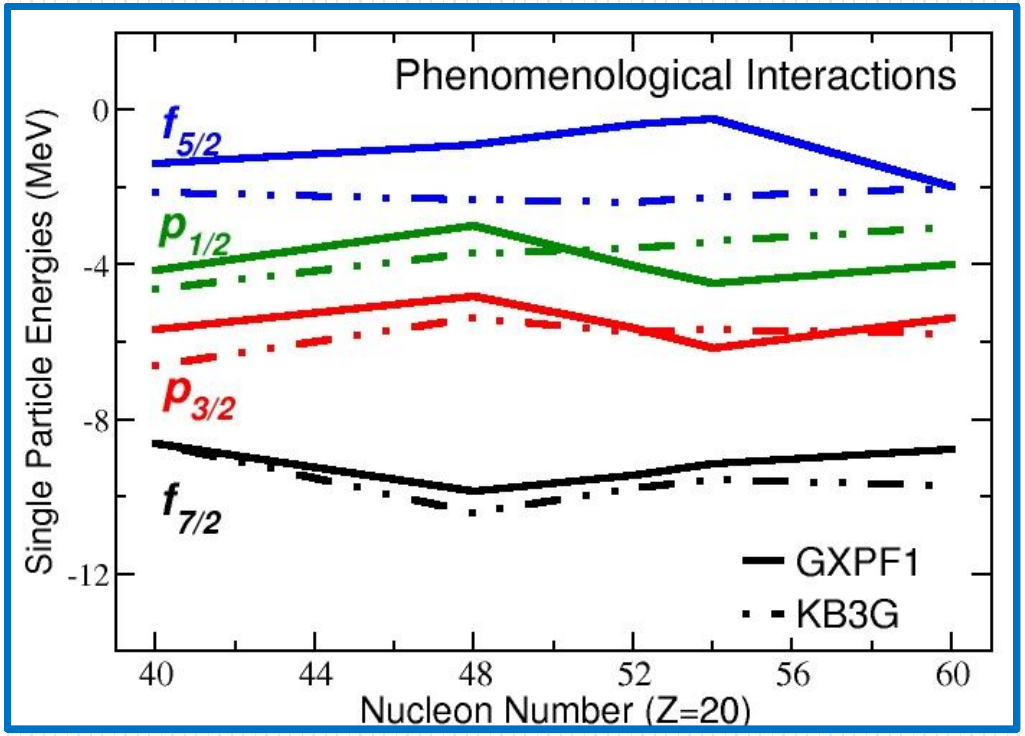
Large $f_{7/2}$-$p_{3/2}$ gap in phenomenological interactions gives shell closure at ^{48}Ca – famously missing with NN-only

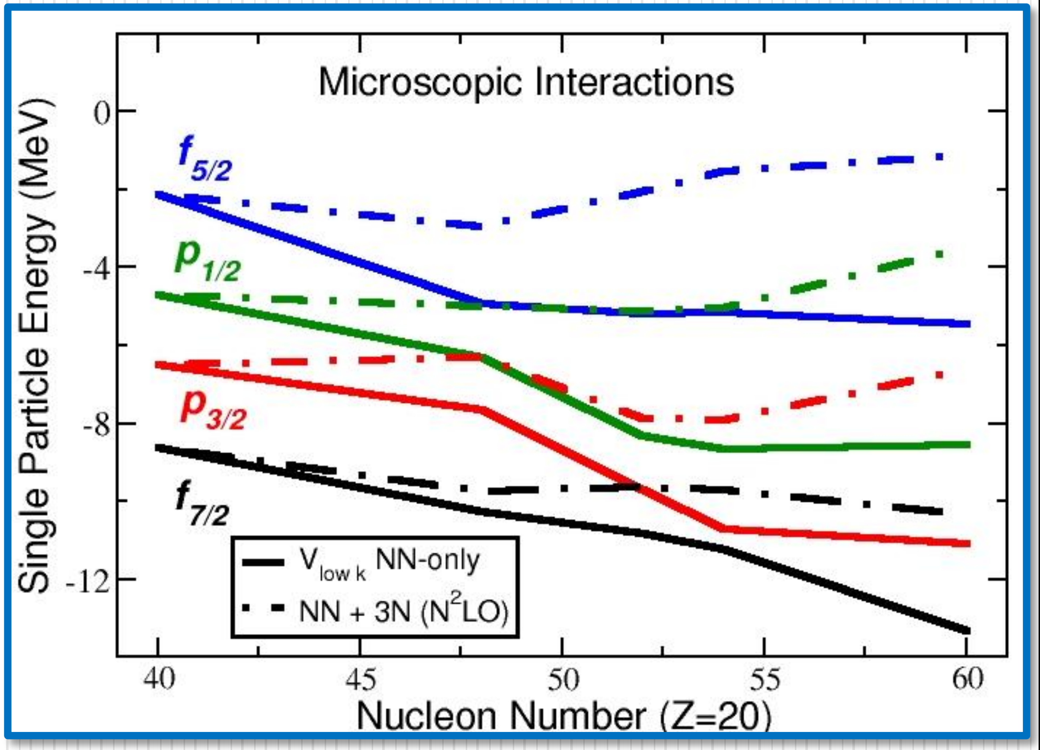
Increase in gap due to 3NF monopoles: indicates enhancement of closed-shell features at ^{48}Ca

Calcium Effective Single Particle Energies

Using GXPF1 SPEs, MBPT with 3 major shells (preliminary)

Calculate SPEs with 3N force monopoles





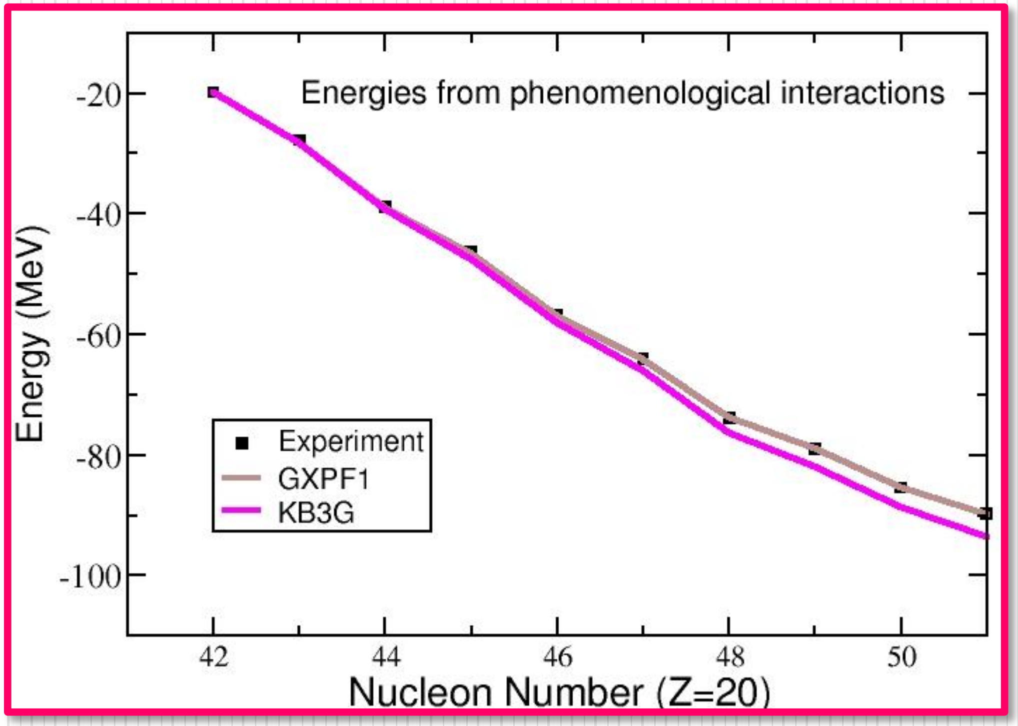
N=34 shell gap: GXPF1 shows closed shell at N=34 – in disagreement with KB3G

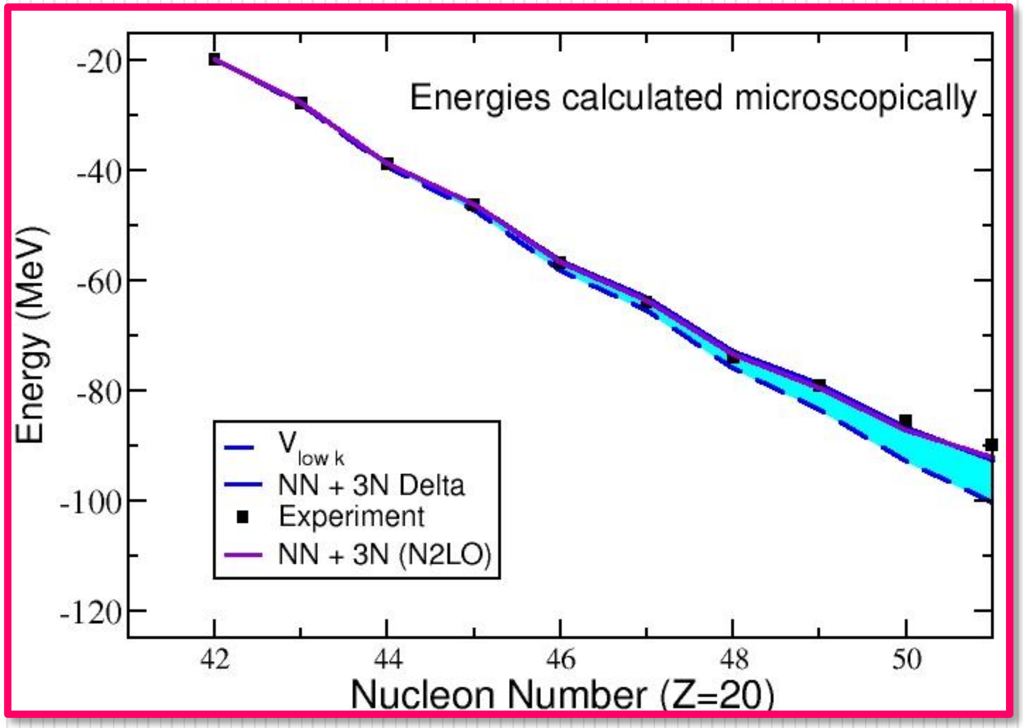
$V_{low\ k}$ also gives gap at N=34, retained after adding 3N – supports GXPF1

Ground State Energies in Ca Isotopes

Perform shell model calculations for Ca isotopes using NN + 3N monopoles

Calculate Binding Energies for isotope chain (preliminary)





With 3N monopoles – close to GXPF1 BEs

Expect slightly more binding for higher intermediate states

NN-only comes to overbind Ca isotopes beyond ~^{46}Ca

3N monopoles correct overbinding – good experimental agrement

Outlook

- Exploring frontiers of nuclear structure of medium mass nuclei with 3N forces

- 3NF contribution to sd- and pf-shell monopoles
  - **Repulsive shift** seen in T=1 monopoles

- **In progress**: T=0 – need 3N effects to **2nd order**

- Correctly predicted binding energies of oxygen isotopes – including dripline
- First calculations in pf-shell with calcium binding energies
- Investigate effects of 3NF on SM interactions as orbits are filled.

Thanks to Collaborators!

A. Schwenk

T. Otsuka

T. Suzuki