Three-Nucleon Forces for Medium-Mass Neutron-Rich Nuclei

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TRIUMF

OAK RIDGE NATIONAL LABORATORY

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Outline

- **Microscopic Theory for Valence Shell Effective NN Interactions**
  - Many-body perturbation theory: methods and interactions
  - Deficiencies: revealed in monopole interaction, oxygen properties
- **3N forces**
  - Chiral Effective Field Theory
  - Inclusion in valence-shell interactions: 1- and 2-body parts
- **Impact on Nuclear Structure**
  - **2-body 3N**: monopole components of valence-shell interaction
  - Evolution of single particle energies (SPE): dripline in oxygen isotopes
  - **1-body 3N**: contribution to microscopic *sd*-shell SPE
    - Parameter-free shell model calculations: impact on spectra

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: $H\psi = E\psi$

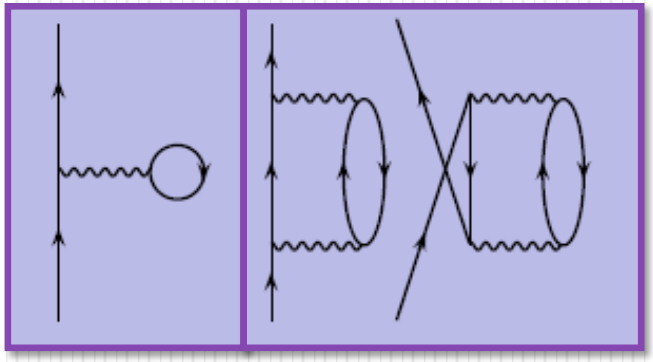
- Impossible to solve in heavy systems in complete Hilbert space

- Consider problem in truncated (model) space defined by projection operator P:

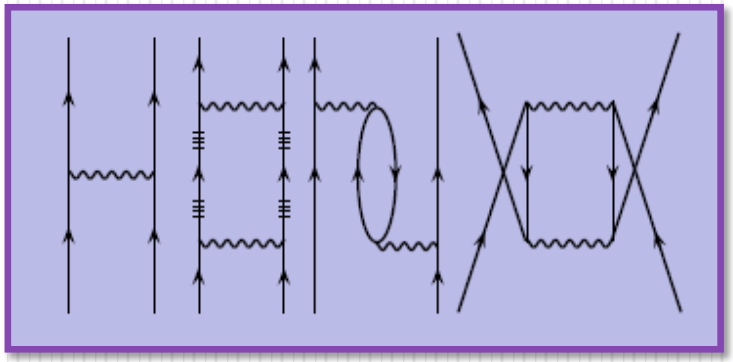
$$PH_{eff}P\psi = EP\psi; \quad H_{eff} = H_0 + V_{eff}$$

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

Folded-diagrams: method to construct effective interaction perturbatively



1-body to 2nd order



2-body to 2nd order

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 a particular set of two-body matrix elements (TBME):

Angular average of interaction

Determines interaction of orbit *a* with *b: evolution of orbitals*

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

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

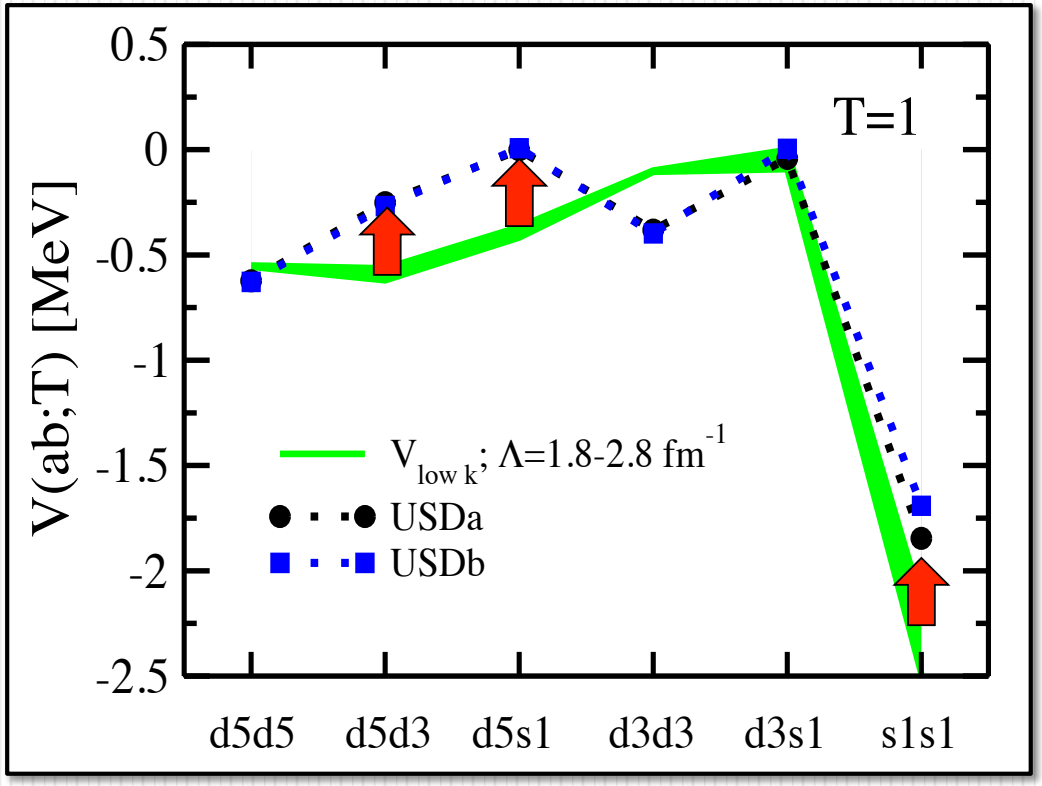
***sd*-shell**: 63 TBME - USD (1984), USDa, USDb (2006)

- global fit of single particle energies (SPEs) and two-body matrix elements; monopoles most important

***pf*-shell:** 195 TBME

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

Phenomenological vs. Microscopic



Compare monopoles from:

- *Microscopic* **low-momentum** interactions
- *Phenomenological* **USD** interactions

Clear shifts for *low-lying orbitals*:

- T=1 repulsive shift

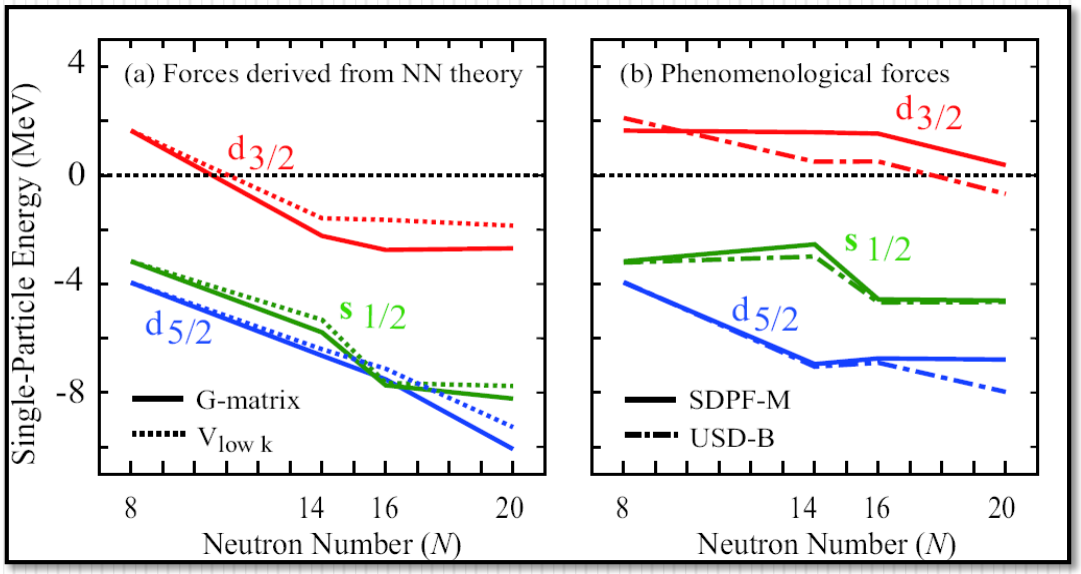
Incorrect hierarchy for $d_{5/2}$-$d_{5/2}$ vs. $d_{5/2}$-$d_{3/2}$

** Origin of the shifts: Can neglected 3N forces explain this?

-- Proposed by **A. Zuker (2003)**

Physical Implications in Oxygen

Monopoles drive *evolution* of single particle energies



Phenomenological Forces

Large gap for ^{22}O

$d_{3/2}$ orbit is unbound

Microscopic NN Theory

No shell gap at ^{22}O

→ Compressed spectra

$d_{3/2}$ orbit is strongly bound

→ Implications for dripline

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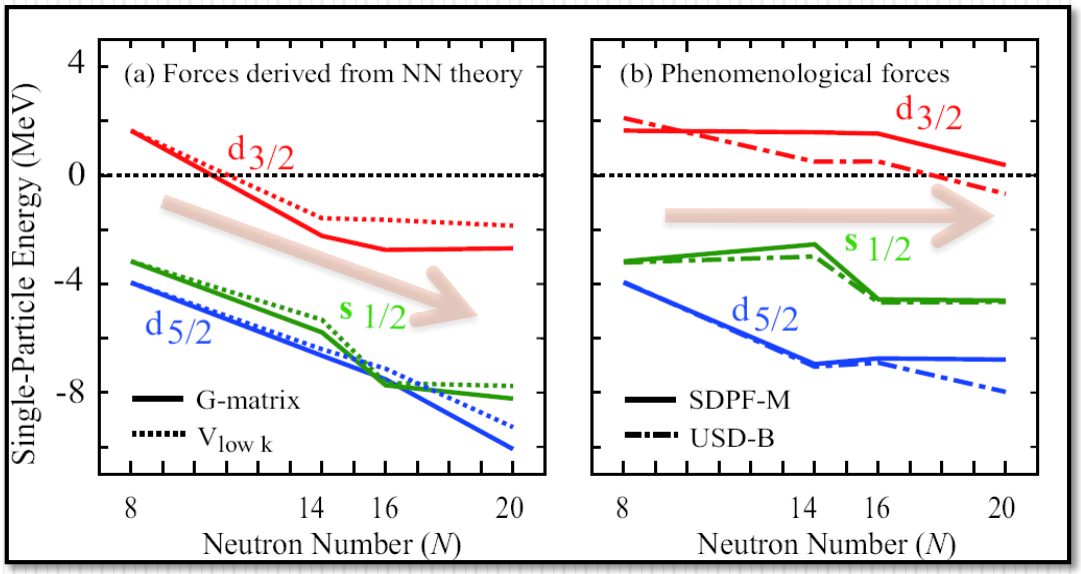

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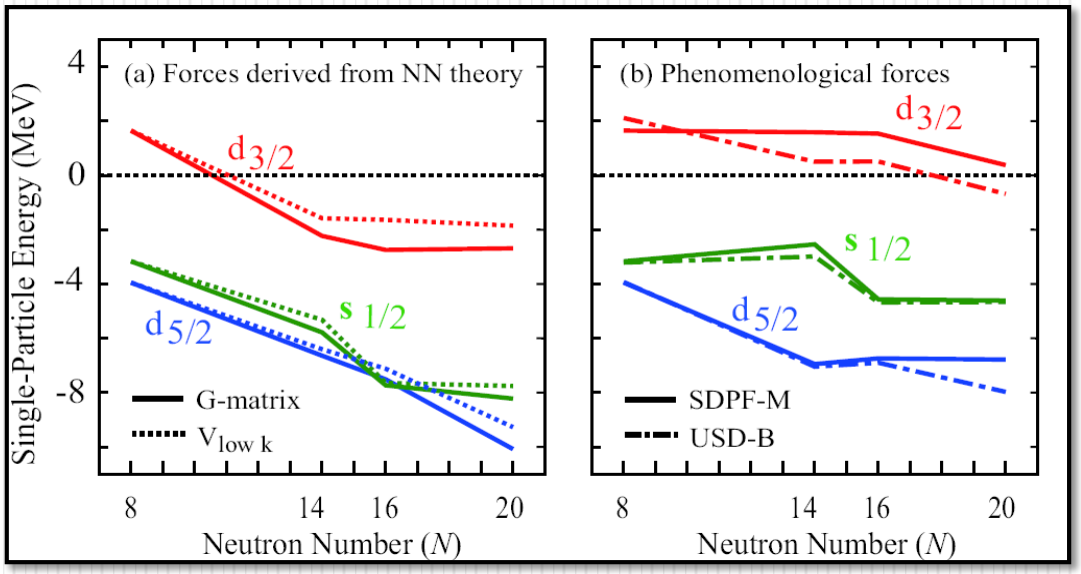

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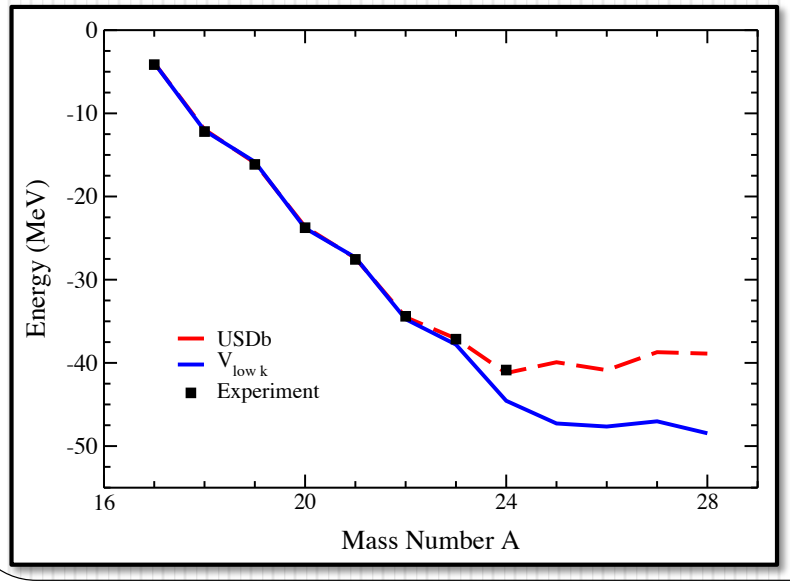

Oxygen: experimentally established dripline at ^{24}O

USDb: O unbound beyond ^{24}O

MBPT: bound through ^{28}O

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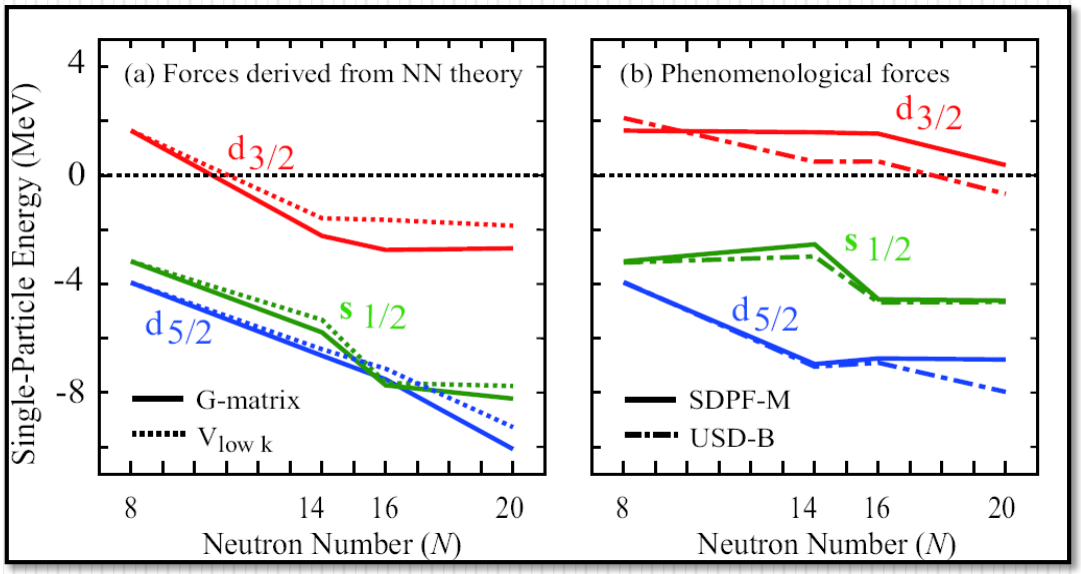

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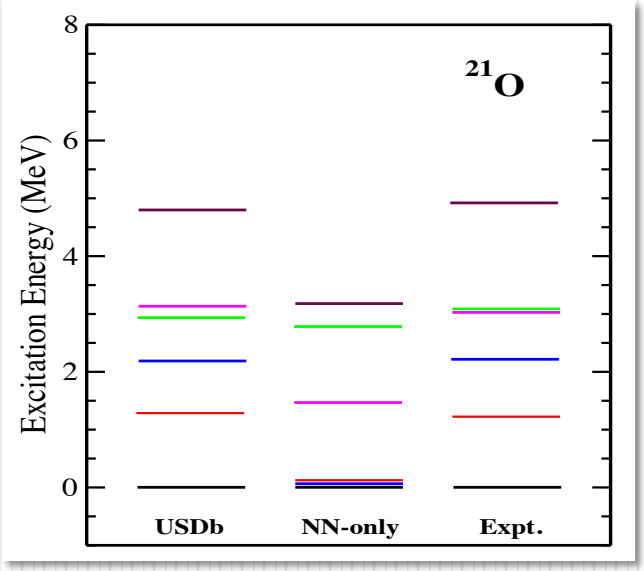

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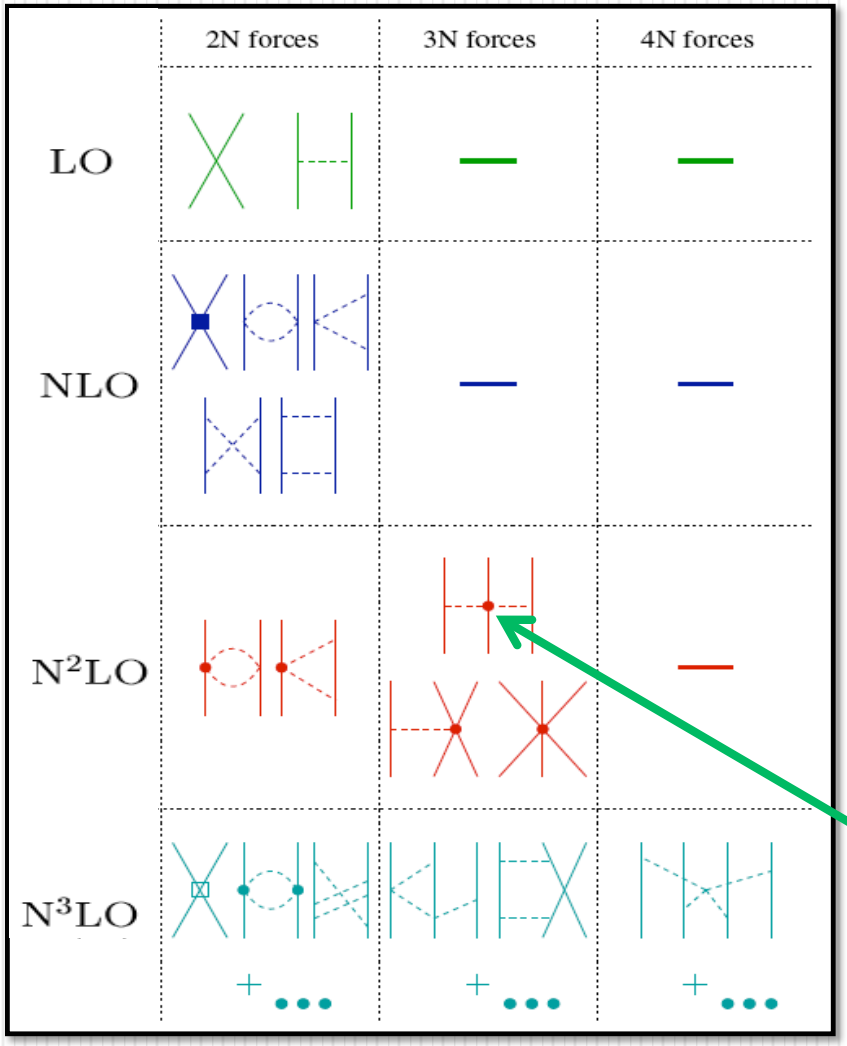
Spectra much too compressed beyond ^{18}O

Chiral Effective Field Theory



Nucleons interact via π exchange and contact interactions

Explains hierarchy: $V_{NN} > V_{3N} > \ldots$

Short-range couplings fit to experiment

Systematic way to include 3NF

Only two new couplings at N²LO:

c terms: already constrained by NN, πN data

$$c_1 = -0.9^{+0.2}_{-0.5},\ c_3 = -4.7^{+1.2}_{-1.0}$$
$$c_4 = 3.5^{+0.5}_{-0.2}$$

No new couplings at N³LO N⁴LO

Chiral 2N: large cutoffs not suitable for MBPT – need to renormalize…

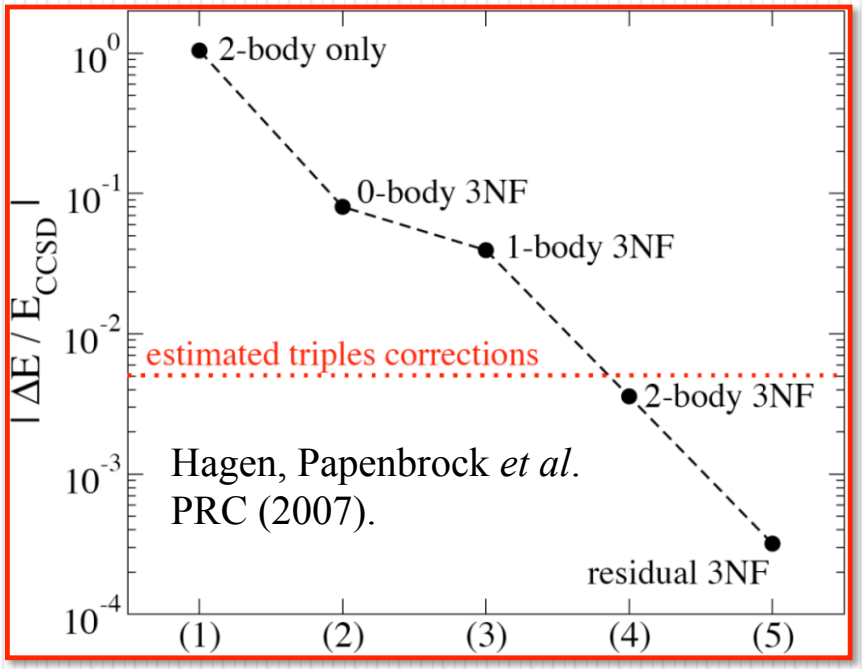
Evolve to lower cutoff using **RG methods** (smooth regulator):

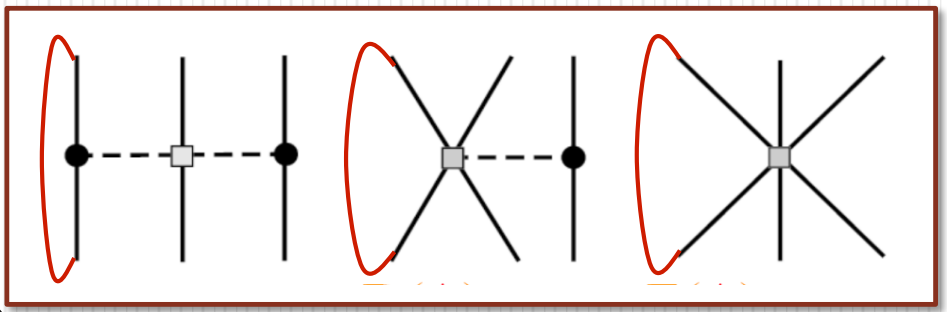
3N Forces for Valence-Shell Theories

$V_{low\ k}(\Lambda)$ + N^{2}LO Chiral $V_{3N}(\Lambda)$

D(Λ), E(Λ) couplings fit in light systems

Approach: inspired by benchmark **Coupled Cluster** results for ^{4}He with 3N





0- 1- and 2-body parts (summed over occupied states) of 3NF dominate:

Neglect residual 3NF

Generate **effective two-body** force from 3N by similar sum (as in nuclear matter)

$$\langle ab | V_{3N,\mathrm{eff}} | a'b' \rangle = \sum_{\alpha=core} \langle ab\alpha | V_{3N} | a'b'\alpha \rangle$$

3N Forces for Valence-Shell Theories

$V_{low\ k}(\Lambda)$ + N^{2}LO Chiral $V_{3N}(\Lambda)$

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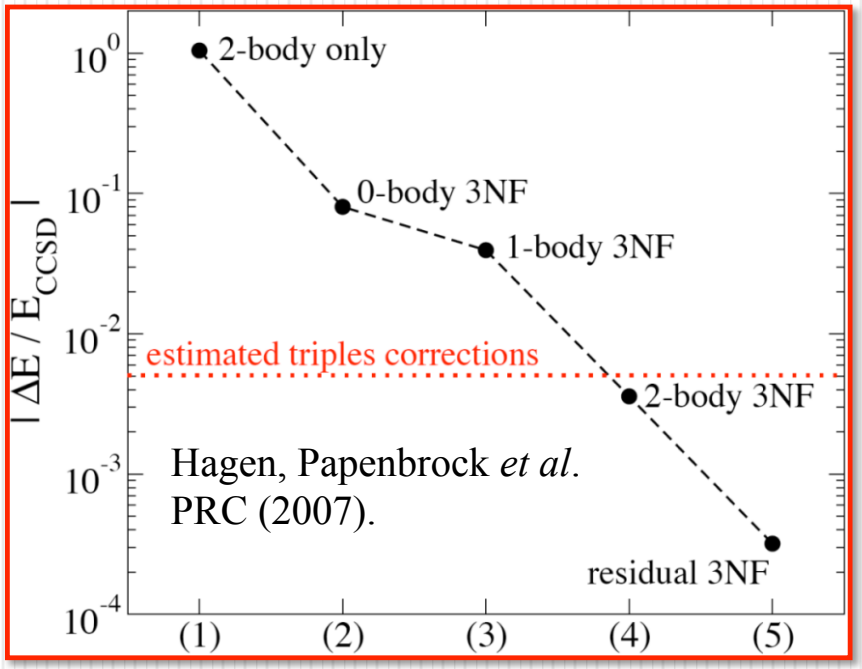

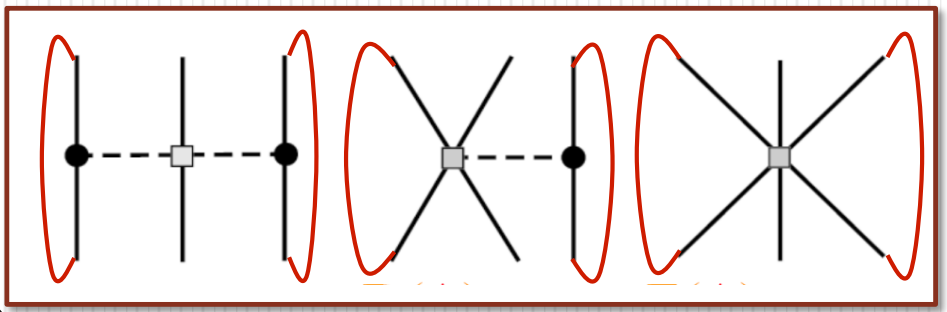

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$$\langle ab|V_{3N,\mathrm{eff}}|a'b'\rangle = \sum_{\alpha=core}\langle ab\alpha|V_{3N}|a'b'\alpha\rangle$$

Effective one-body contribution:

$$\langle a|V_{3N,\mathrm{eff}}|a'\rangle = \frac{1}{2}\sum_{\alpha\beta=core}\langle a\alpha\beta|V_{3N}|a'\alpha\beta\rangle$$

- 3N forces tractable in shell model

Calculation Details

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

1 NN matrix elements derived from:

- Chiral N^{3}LO (Machleidt, 500 MeV) using smooth-regulator $V_{\text{low } k}$ with range of cutoffs
- 3rd-order in MBPT
- $20\hbar\omega$ intermediate state configurations (converged)

2 3N forces: calculate monopole components from:

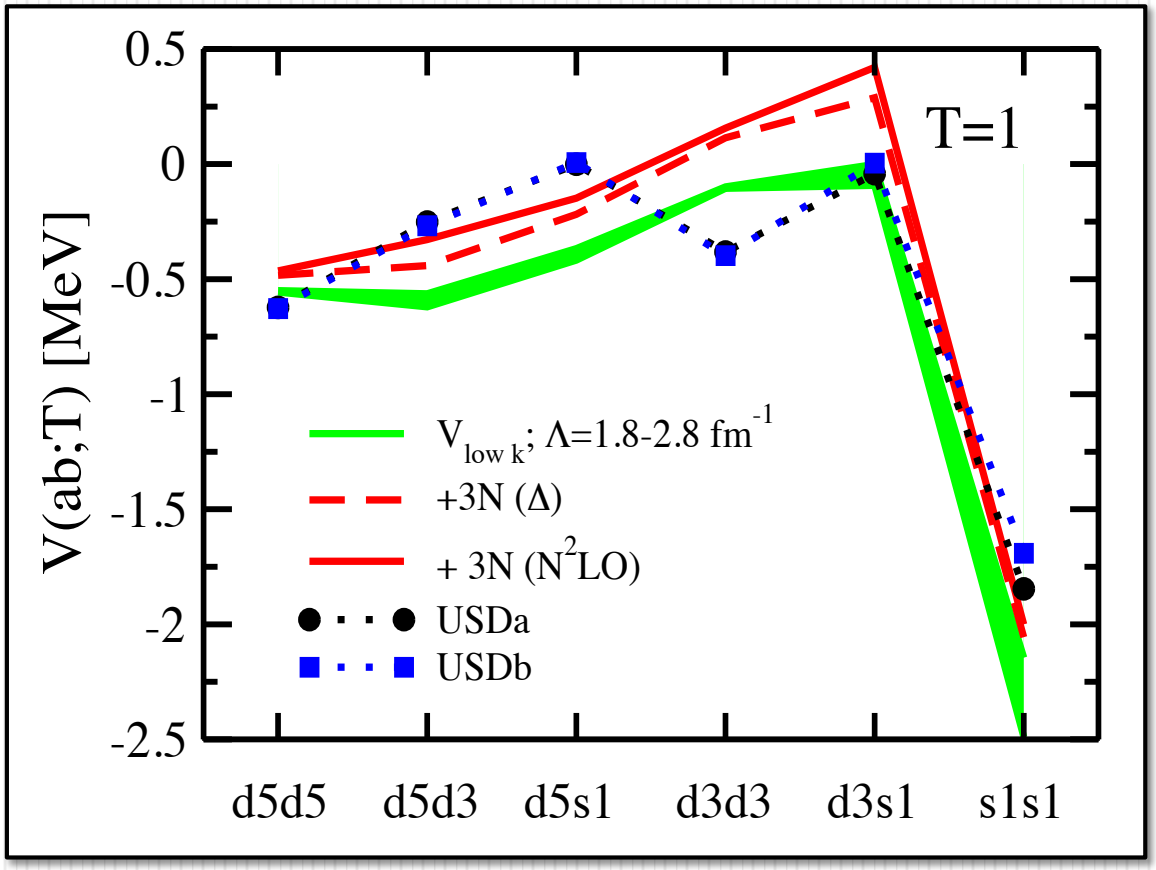
A) Chiral N^{2}LO fit to above $V_{low\ k}$ with $\Lambda = 2.0$ fm^{-1}

B) One-Delta excitation from N^{2}LO: specific choice of ***c*-terms**

Converged in 3NF partial waves up to $J \leq \frac{7}{2}$

Included to **first order** in perturbation theory

Two-body 3N: Monopoles in *sd*-shell

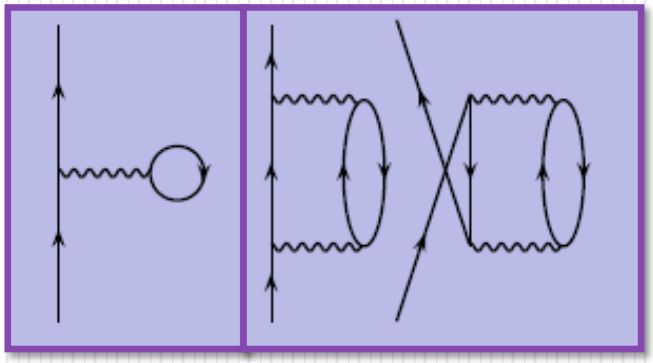


- Dominant effect from **one-Δ** – as expected from cutoff variation
- 3N forces produce clear repulsive shift in monopoles

- First calculations to show missing monopole strength due to neglected 3N
- Restores monopole hierarchy $d_{5/2}$-$d_{5/2}$ vs. $d_{5/2}$-$d_{3/2}$
- **Future**: Improved treatment of high-lying orbits – treat as holes in ^{40}Ca core

One-body 3N: Calculation of SPEs

So far phenomenological SPEs: NN-only microscopic SPE yield "poor" results



- *sd*-shell: Self-consistent calculation in MBPT $20\hbar\omega$ (converged) to 3rd-order
- NN-only insufficient: consistent with similar studies (Coraggio, *et. al*, 2007)

Orbit	"Exp"	USDb	NN
$d_{5/2}$	-4.14	-3.93	-5.43
$s_{1/2}$	-3.27	-3.21	-5.32
$d_{3/2}$	0.944	2.11	-0.97

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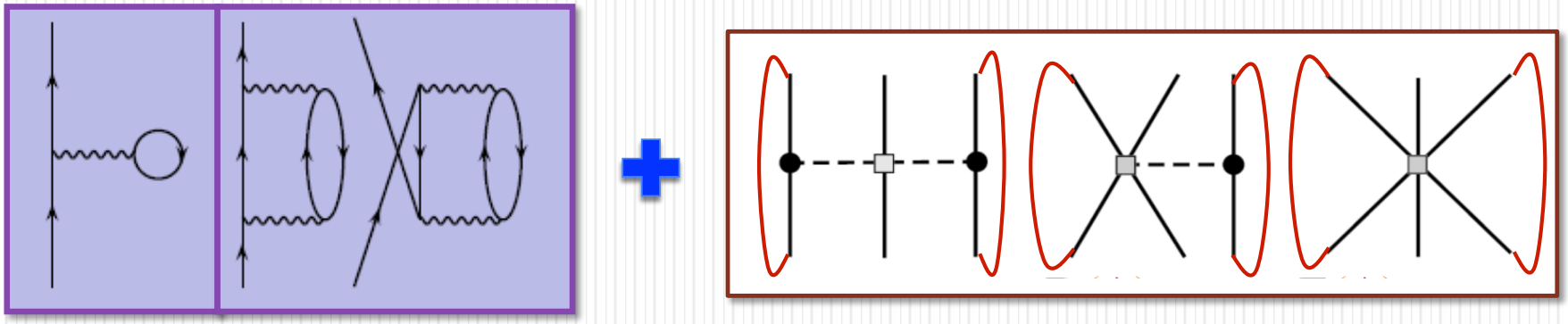

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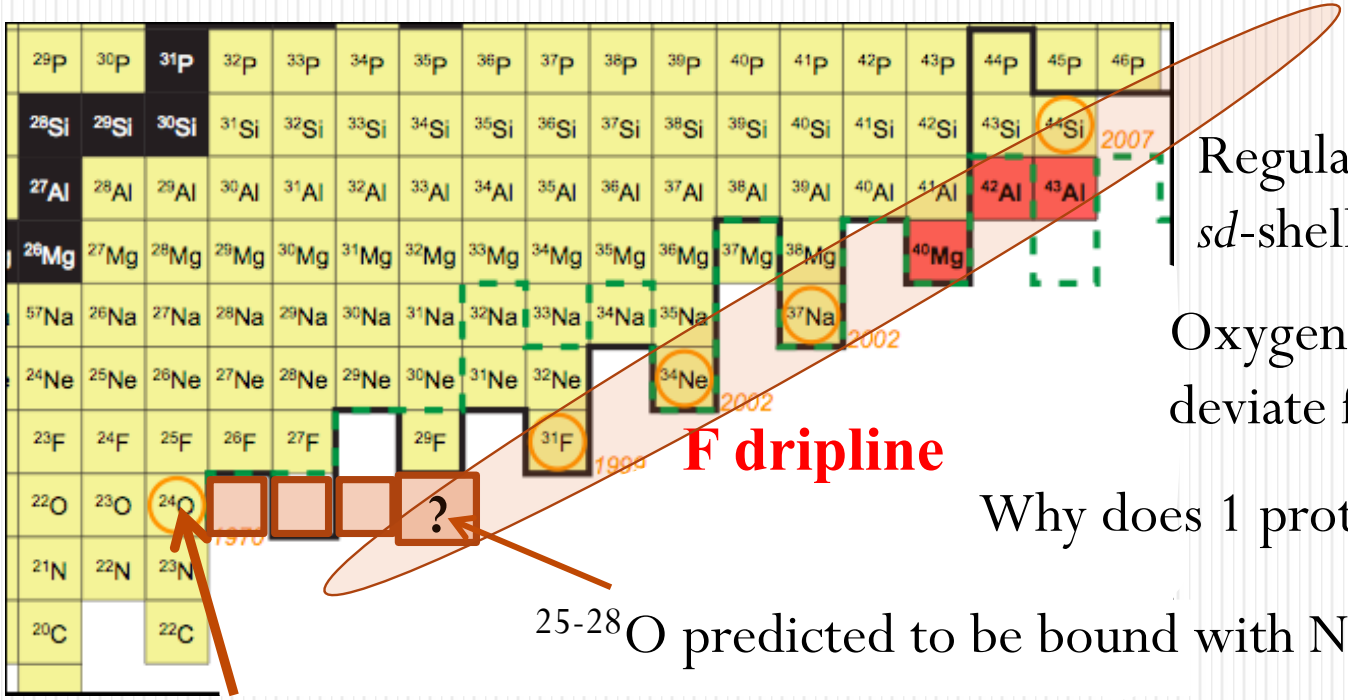
Orbit	"Exp"	USDb	NN	3N	NN+3N
$d_{5/2}$	-4.14	-3.93	-5.43	1.36	-4.07
$s_{1/2}$	-3.27	-3.21	-5.32	3.39	-1.93
$d_{3/2}$	0.944	2.11	-0.97	3.06	2.09

- Consistent with CC hierarchy: 1-body 3N > 2-body 3N ~ order of magnitude
- Microscopic SPEs: Reasonable agreement with USD, experimental

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?

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

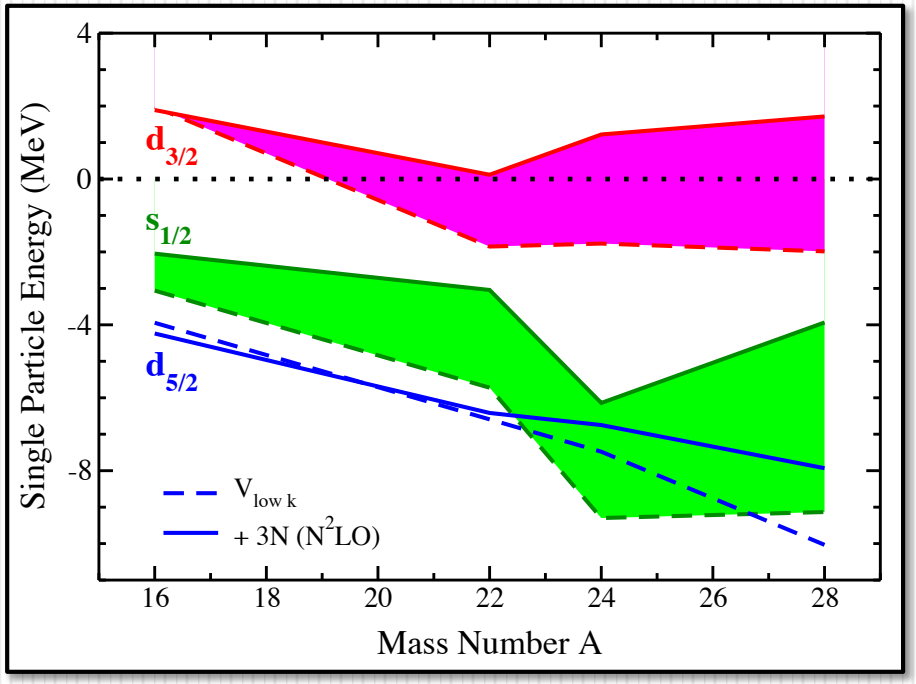
Experimental Oxygen dripline observed at ^{24}O

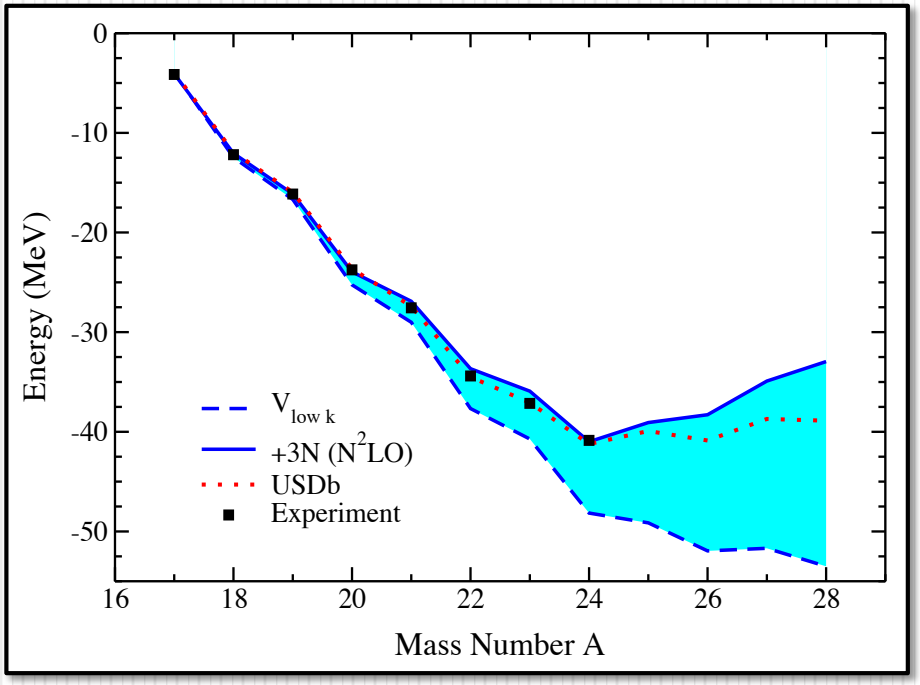
Monopole changes multiplied by neutron number – small changes will impact neutron-rich regions

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

Fully-Microscopic Calculations

- Does the same conclusions hold when using microscopic SPEs?
- Use microscopic NN+3N monopole matrix elements and NN+3N SPEs
- Compare with NN-only MBPT, USD SPEs

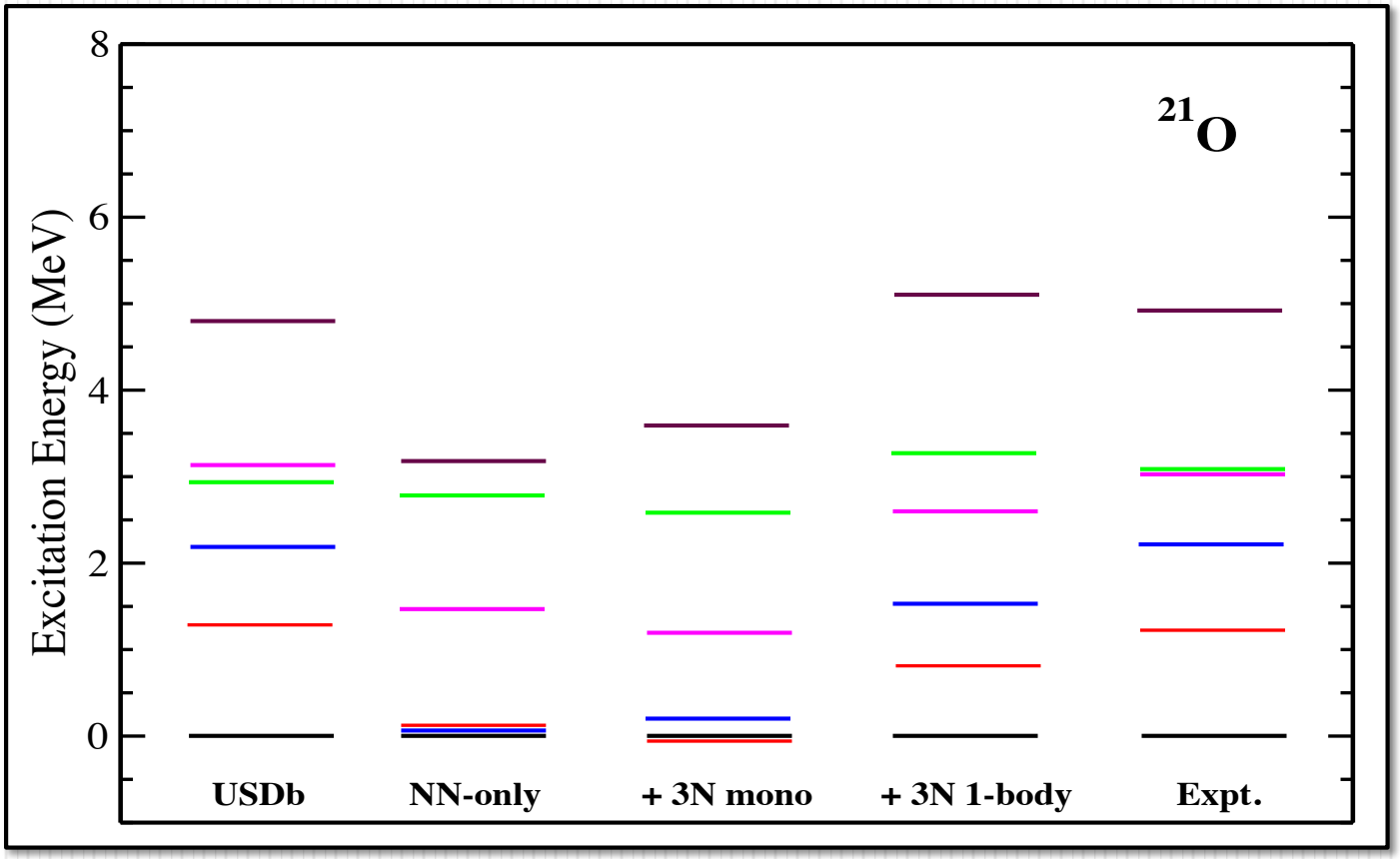




- ***Fully-microscopic*** calculation still predicts dripline at ^{24}O

Impact on Spectra

- ***Fully-microscopic*** calculation of spectra in oxygen isotopes



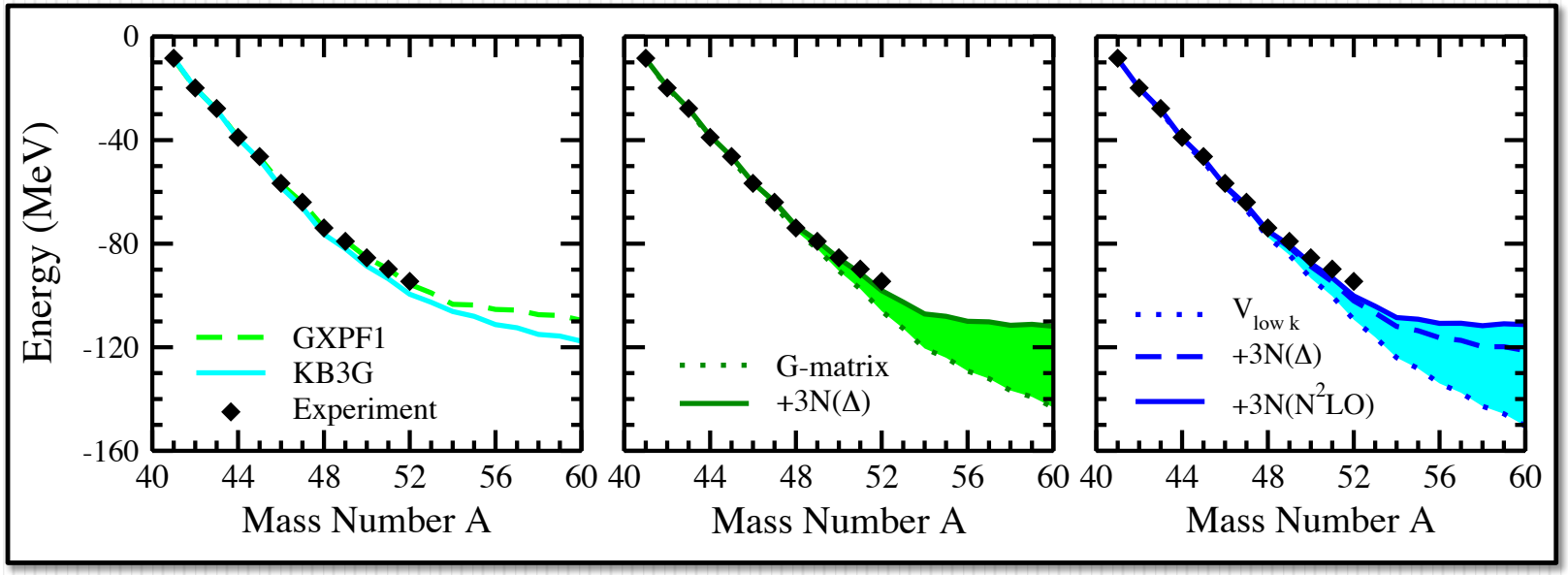
- NN-only: poor agreement with experiment
- 3N monopoles offer some help: spectrum still too compressed
- Using microscopic 3N monopoles, NN+3N SPEs: beneficial for spectrum
  - Correct ordering, improved spacing – need to include full 3N multipoles

Ground State Energies in Ca Isotopes

Include many-body correlations by diagonalization in model space

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

Calculate binding energies for isotope chain



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

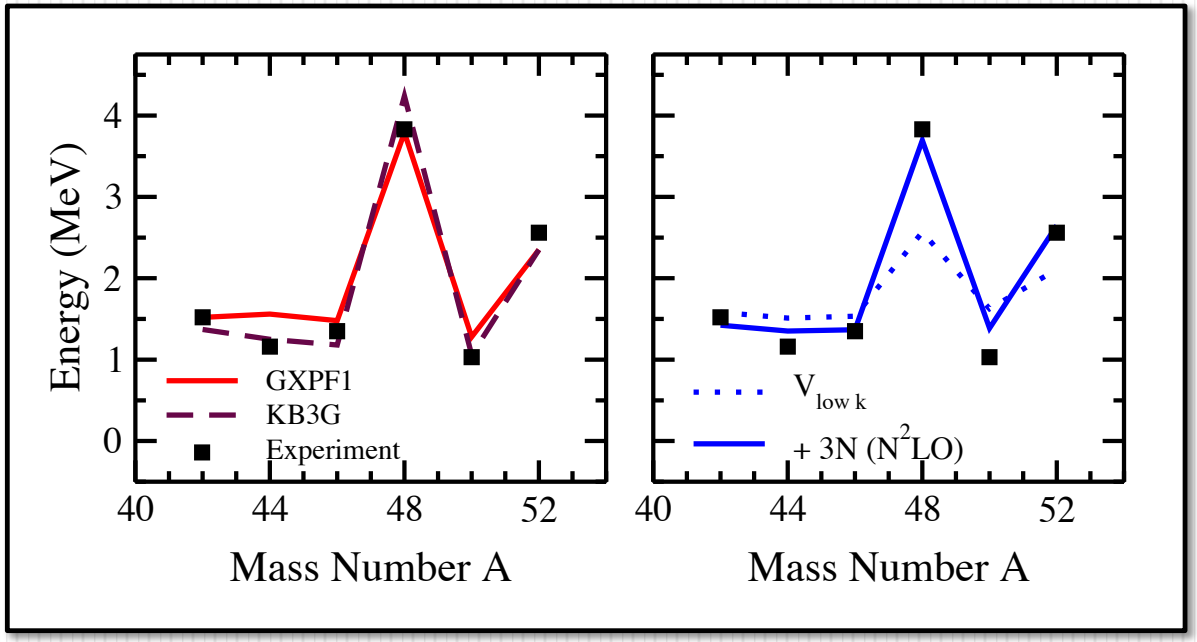
3N forces correct overbinding: good experimental agreement

Correction from 3N Δ consistent between methods

Shell Gap in ^{48}Ca

Shell gap in ^{48}Ca well-reproduced with phenomenological interactions

Calculate first 2^+ excited states in calcium isotopes



3N forces: improvement of ^{48}Ca 2^+ energy ~1 MeV

Cures another NN-only failing: can reproduce ^{48}Ca shell closure

Strongly dependent on SPE chosen

- Remove ambiguity: calculate microscopically with 3N, as in *sd*-shell

Outlook

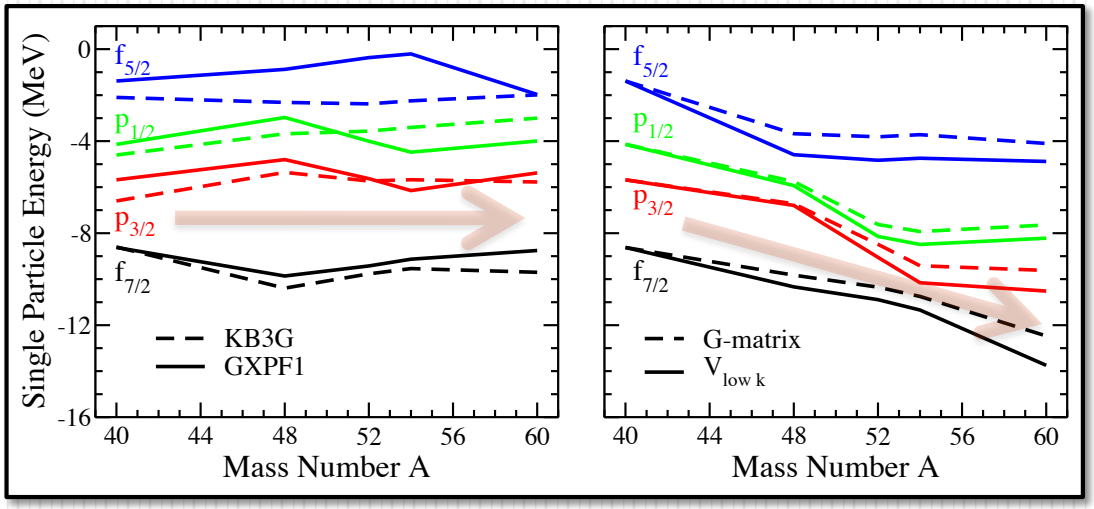
- Exploring frontiers of nuclear structure of medium-mass nuclei with 3N forces
- **2-body 3NF**: contribution to TBME – monopoles
  - **Repulsive shift** seen in T=1 monopoles due to 3N forces in *sd*- and *pf*-shells
- First shell model results in *sd*-, *pf*-shells using chiral 3N forces:
  - Leads to correct predicted binding energies and evolution of shell structure
  - Cures NN-only failings: Dripline, spectra in oxygen, shell gap in ^{48}Ca
- **1-body 3NF**: Microscopic SPEs in *sd*-shell – parameter-free shell model calculations
- **In progress**:
  - Microscopic SPEs in *pf*-shell
- **Near Future**:
  - T=0: need NN-3N to **2nd order**
  - Ni, Sn Isotopes
  - Continuum effects near driplines with K. Tsukiyama (Tokyo)

Thanks to Collaborators: T. Otsuka , A. Schwenk, T. Suzuki

Travel support from UNEDF

Physical Implications in Calcium

Monopoles drive *evolution* of single particle energies



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Large gap at ^{48}Ca

Trend across

Shell gap at ^{54}Ca?

Microscopic NN Theory

Smaller gap at ^{48}Ca

→ Compressed spectra

Trend down

$f_{5/2}$ orbit is strongly bound

→ Implications for gs energy

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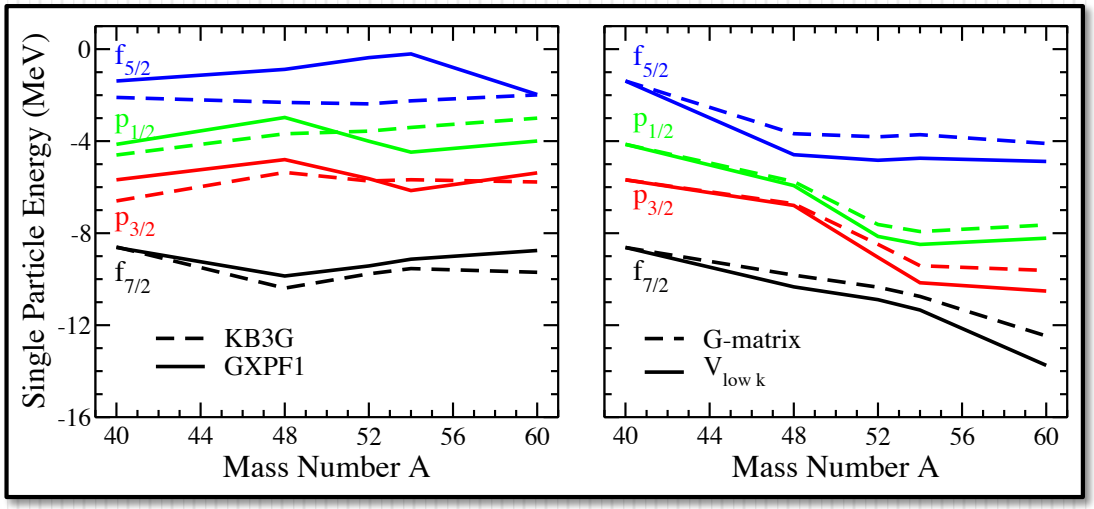
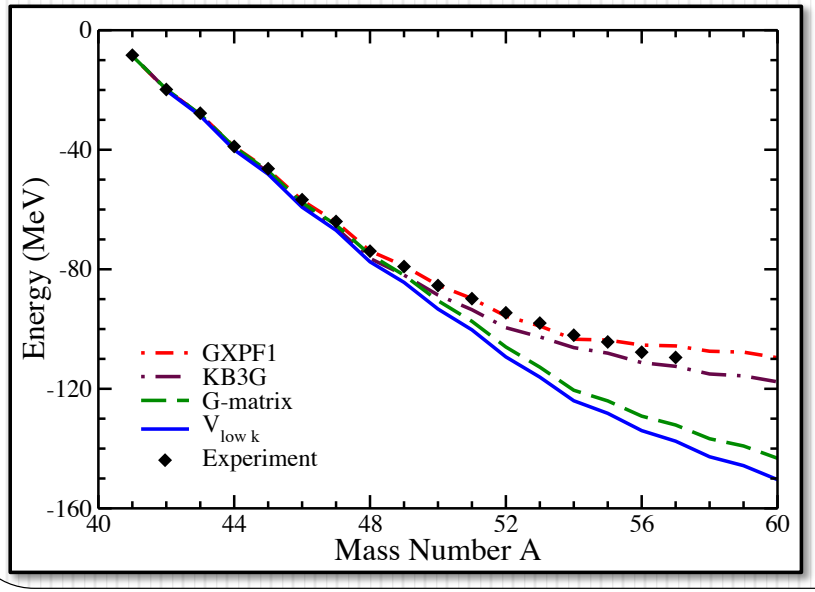


MBPT- Overbind beyond ^{48}Ca



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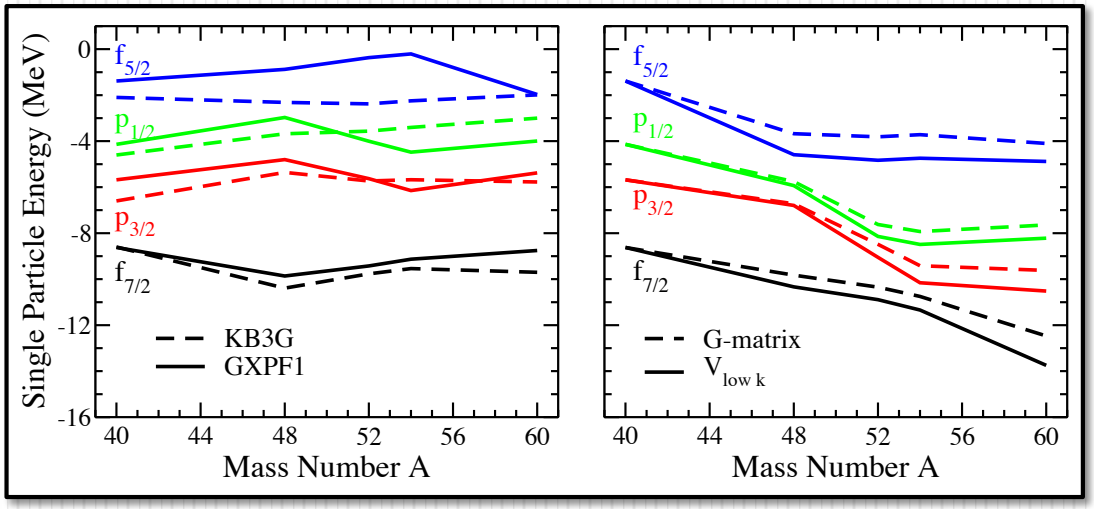
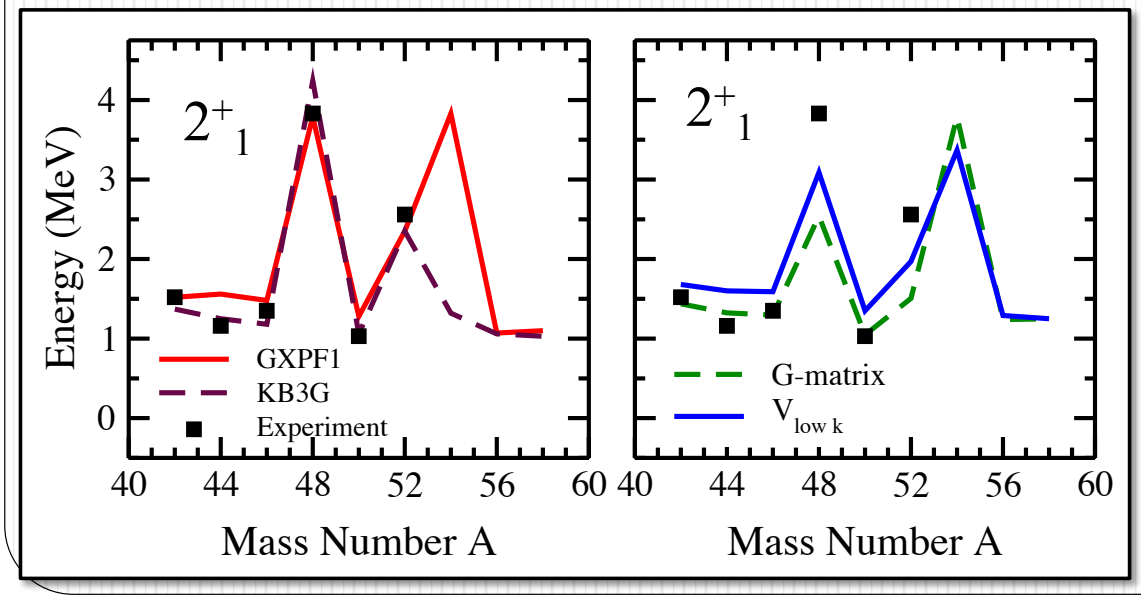


MBPT: No shell closure at ^{48}Ca – failure of NN



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$f_{5/2}$ orbit is strongly bound

→ Implications for gs energy

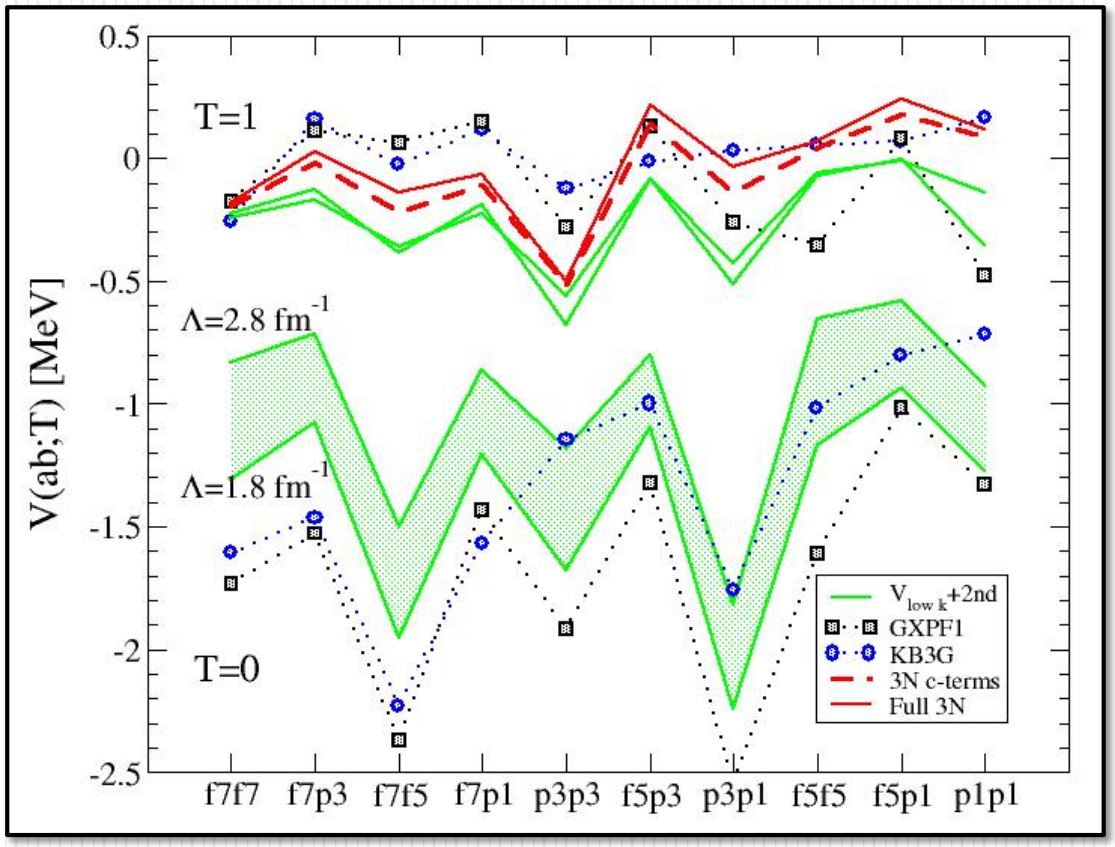
Initial SPE: important factor

If 3N forces explain monopole shifts, should impact BE and shell structure predictions

How can we include them?

Two-body 3N: Monopoles in *pf*-shell

Similar picture as in *sd*-shell

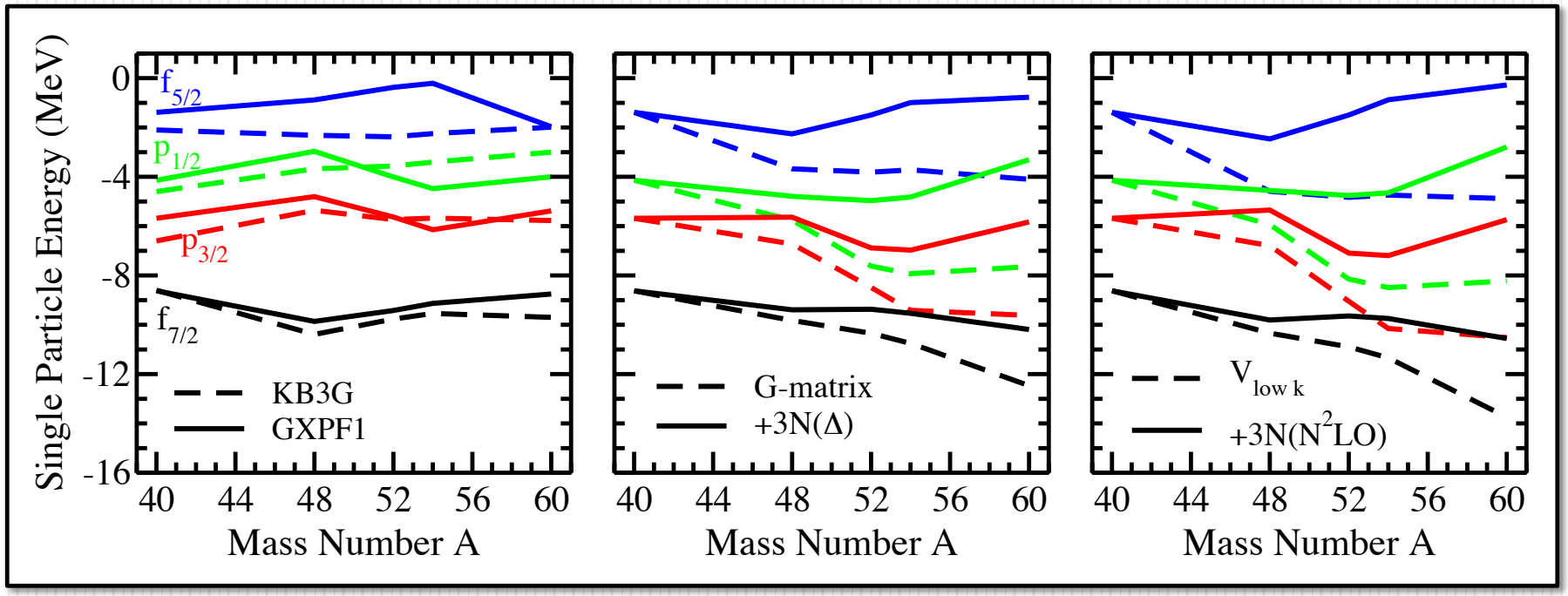


- 3N included to **first order** in MBPT
- Converged in 3NF partial waves up to: $J \leq \frac{7}{2}$
- Dominant effect from **one-Δ** – as expected from cutoff variation
- 3N forces produce repulsive shift in monopoles

T=0: Expect attraction from 2nd order NN-3N interactions: **in progress**

Calcium Effective Single Particle Energies

Calculate SPE evolution with 3N forces

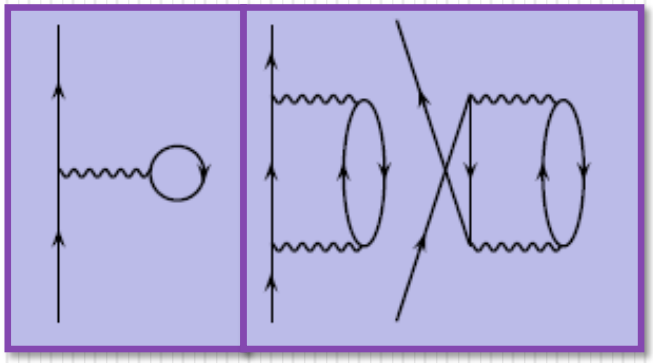


With 3N forces:

- Trend across: improve binding energies
- Increased gap at ^{48}Ca: enhancement of closed-shell features
- N=34 shell gap: robust prediction of shell gap at N=34

One-body 3N: Calculation of SPEs

So far phenomenological SPEs: NN-only microscopic SPE yield "poor" results



- *sd*-shell: Self-consistent calculation in MBPT $18\hbar\omega$ to 3rd-order (converged)
- NN-only insufficient: consistent with similar studies (Coraggio, *et. al*, 2007)

Orbit	"Exp"	GXPF1	NN
$0f_{7/2}$	-8.36	-8.62	-10.77
$1p_{3/2}$	-6.26	-5.68	-10.83
$1p_{1/2}$	-4.46	-4.14	-8.99
$0f_{5/2}$	-1.86	-1.38	-6.47

One-body 3N: Calculation of SPEs

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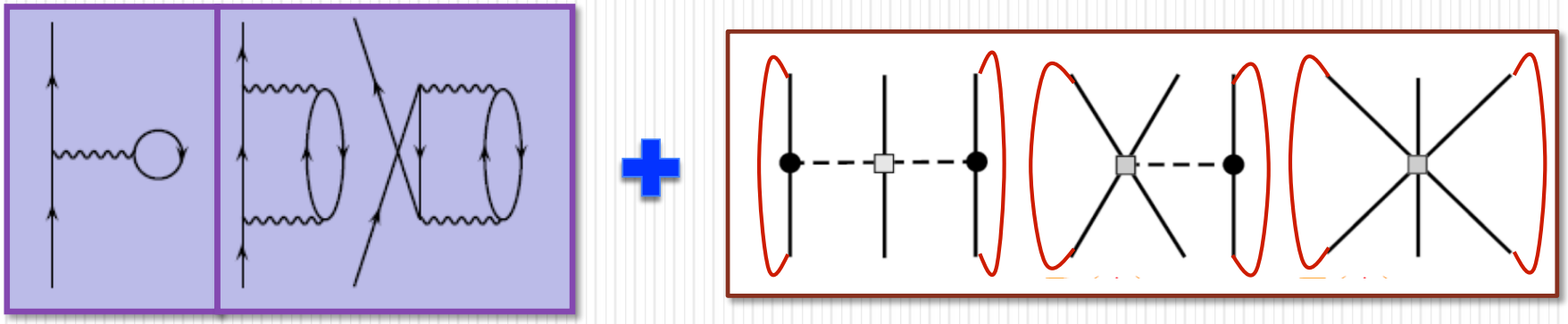


- *sd*-shell: Self-consistent calculation in MBPT $18\hbar\omega$ to 3rd-order (converged)
- NN-only insufficient: consistent with similar studies (Coraggio, *et. al*, 2007)

Orbit	"Exp"	GXPF1	NN	3N	NN+3N
$0f_{7/2}$	-8.36	-8.62	-10.77	2.42	-8.35
$1p_{3/2}$	-6.26	-5.68	-10.83	5.23	-5.58
$1p_{1/2}$	-4.46	-4.14	-8.99	6.17	-2.83
$0f_{5/2}$	-1.86	-1.38	-6.47	4.74	-1.73

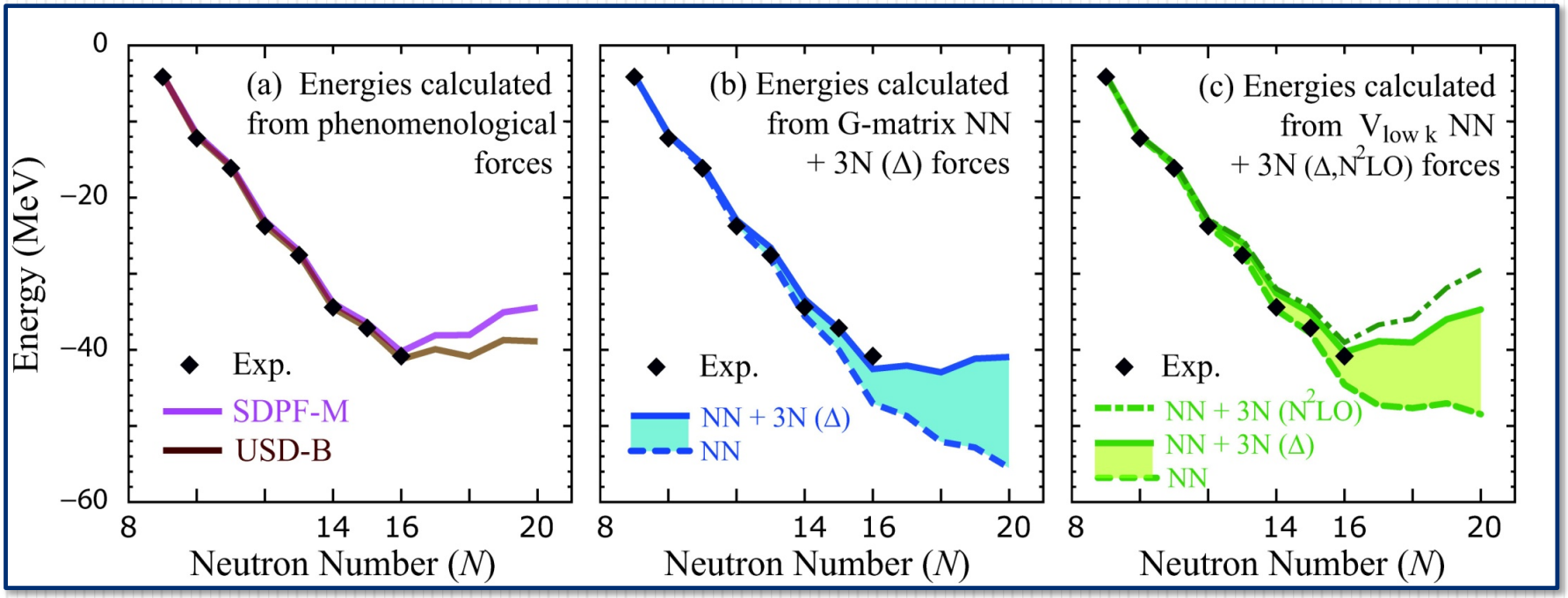
- Consistent with coupled cluster: 1-body 3N > 2-body 3N ~ order of magnitude
- Microscopic SPEs: Reasonable agreement with USD, experimental

Calculated Oxygen Binding Energies

Introduce many-body correlations by diagonalization in model space

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



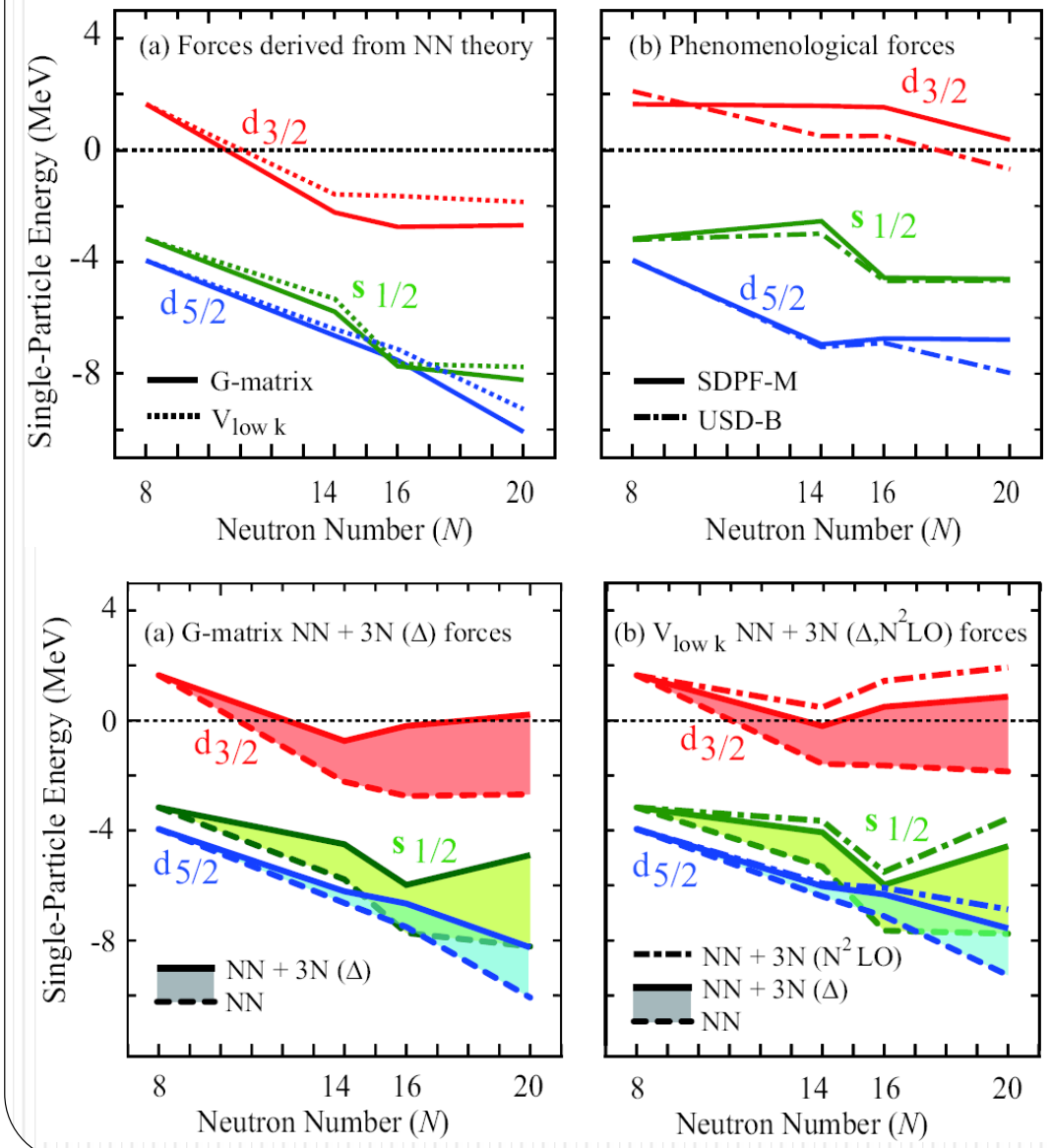
Phenomenological interactions show $^{25\text{-}28}$O less bound than ^{24}O

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

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

Evolution of SPEs in *sd*-shell

First results with 3N forces



$d_{3/2}$ orbit bound for microscopic NN-only interactions

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

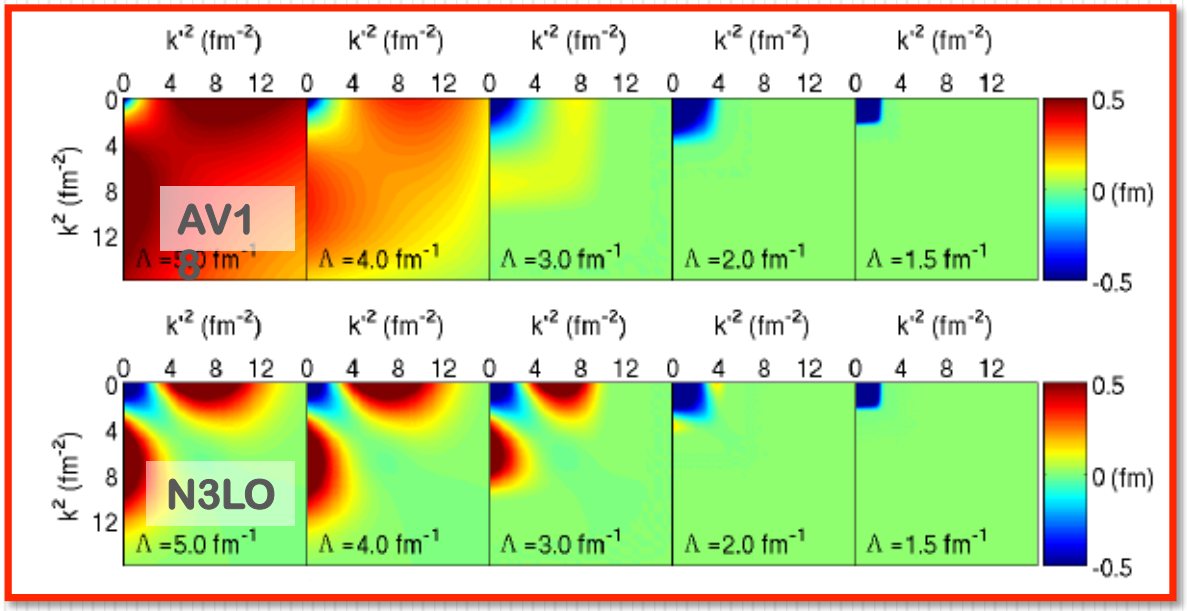
$d_{3/2}$ becomes unbound orbit with addition of 3N forces

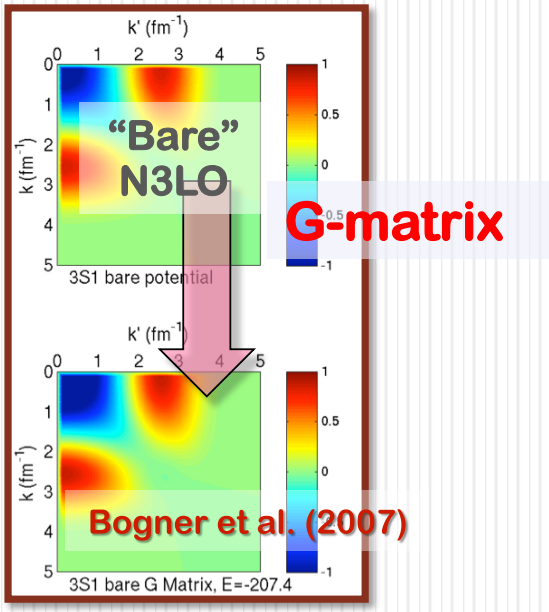
Similar behavior for single Δ and chiral N^{2}LO forces

Nuclear Interactions

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

Chiral interactions provide systematic, consistent 3N





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

Details of Calculation

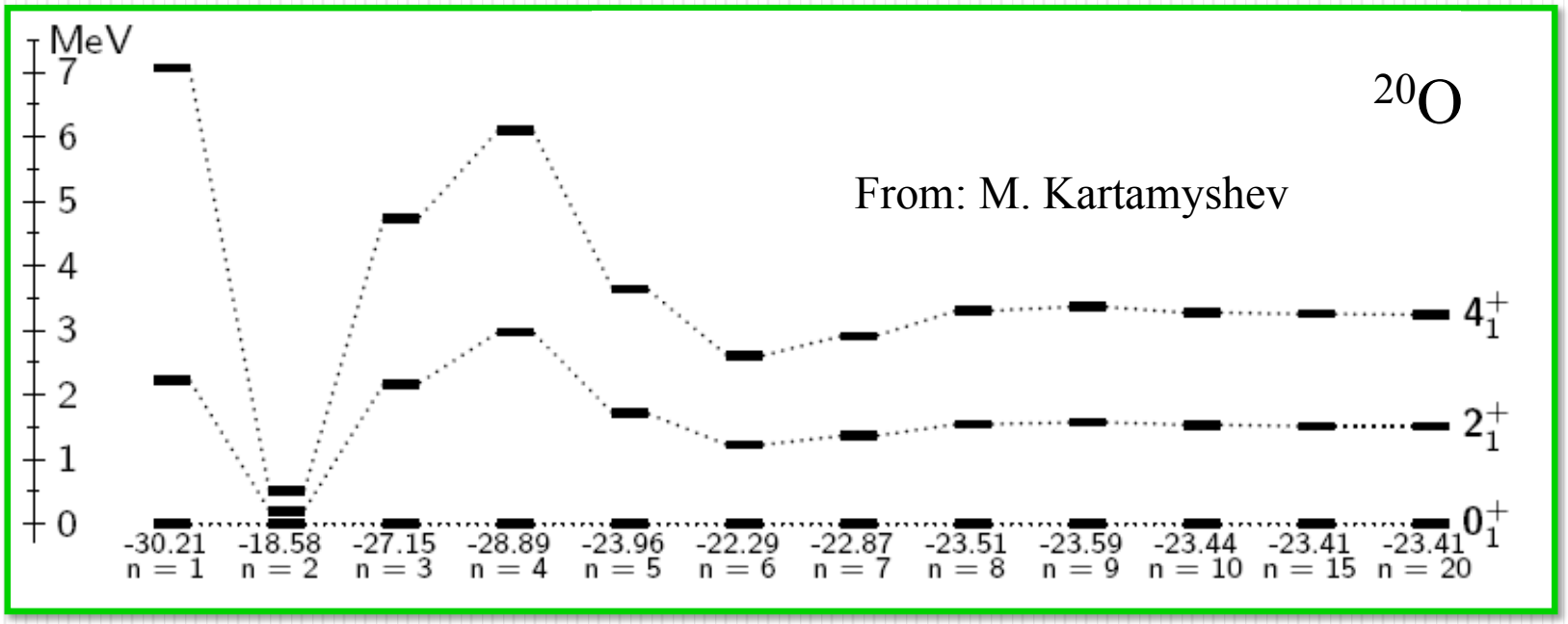
Assume degenerate model space

Intermediate states excitations: 16hw

Neglect 3-body and higher Q-box

FD iterative scheme: converged ~10 iterations

3rd-order in Perturbation Theory



Effective Interaction

Effective interaction given by infinite series of "folded" diagrams:

$$V_{\text{eff}} = \hat{Q} - \hat{Q}' \int \hat{Q} + \hat{Q}' \int \hat{Q} \int \hat{Q} - \hat{Q}' \int \hat{Q} \int \hat{Q} \int \hat{Q} + \ldots$$

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

Several ways to solve the infinite series

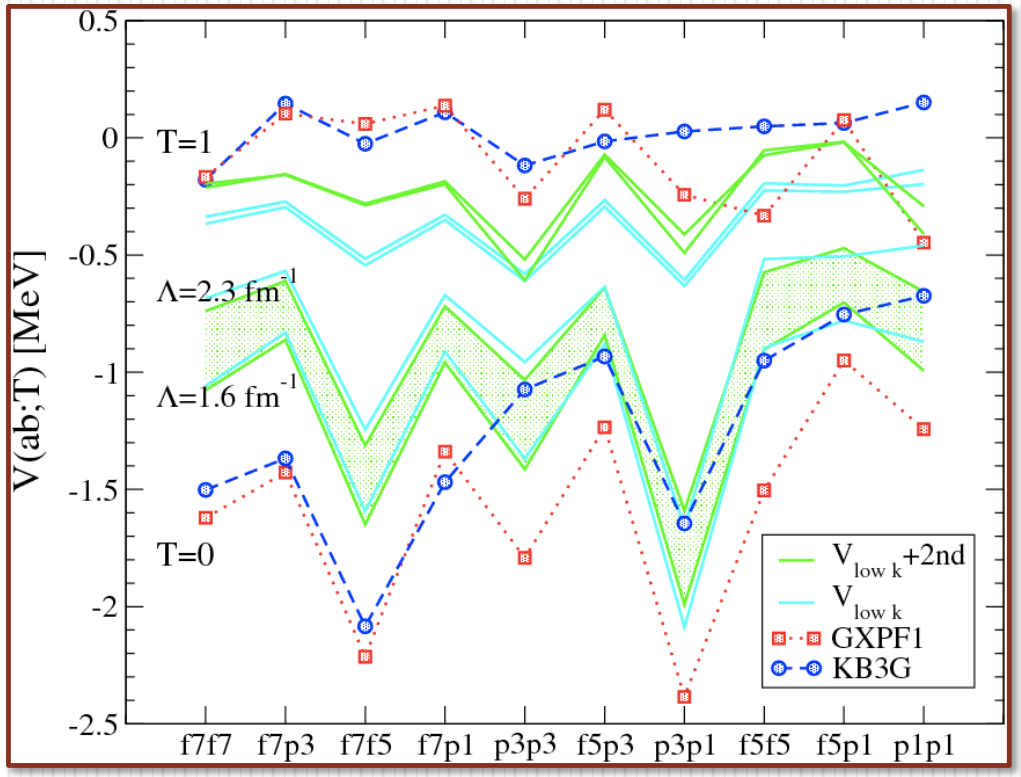
Assuming degenerate model space, $PH_0P = \omega P$, can obtain V_{eff} from Lee-Suzuki iterative scheme:

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

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

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)

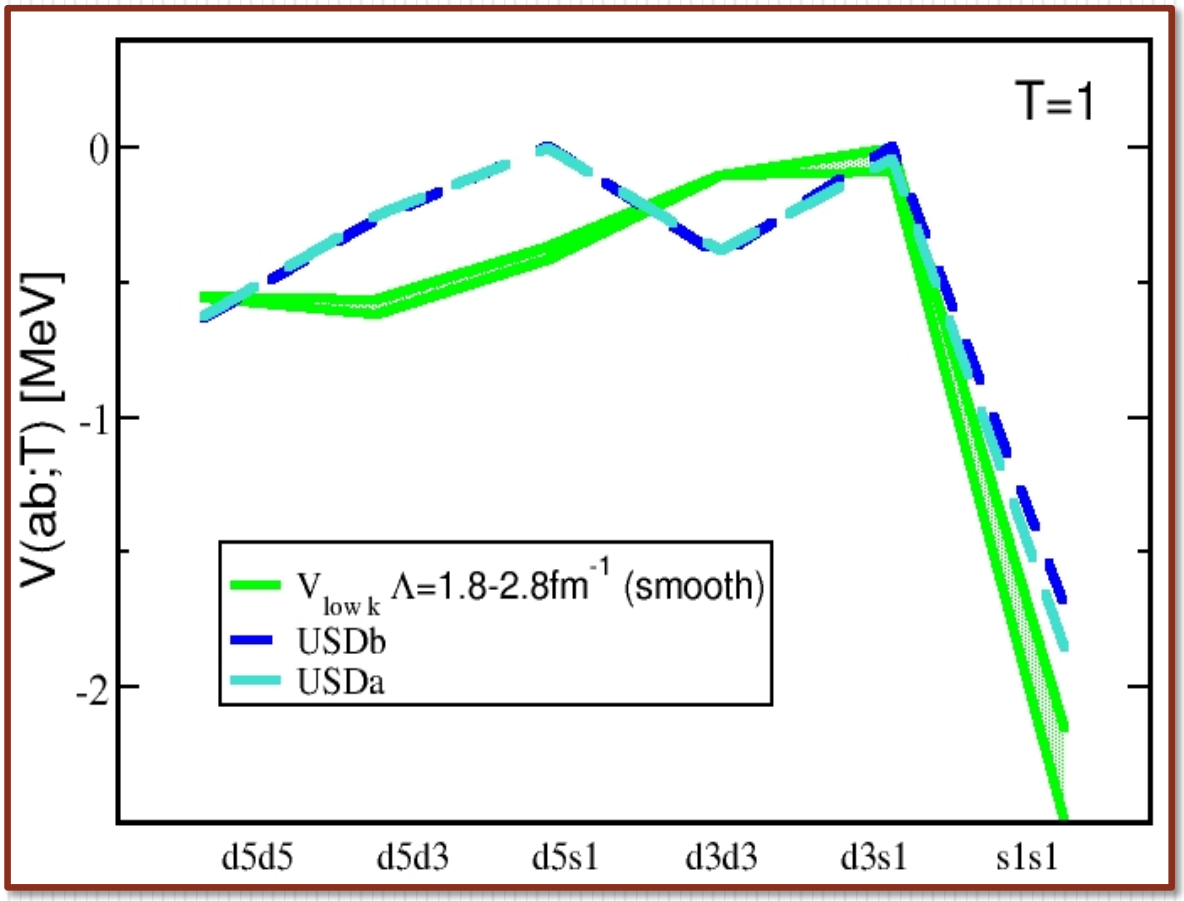
T=0: large cutoff dependence

- Expect attraction from 2nd order NN-3N

- Not enough to calculate effects to first order only for T=0
- Similar trends seen in sd-shell

Cutoff Dependence of Monopoles

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



T=1: cutoff-independent monopoles

- Indicates **c** terms may dominate (repulsive contribution in nuclear matter)
- Wrong hierarchy for low-lying T=1 monopoles with microscopic theory

Many-Body Perturbation Theory

To construct the effective interaction, define $\hat{Q}$-box = sum of all possible topologically distinct diagrams which are irreducible and valence linked:

1-body Q-box to 2nd order

2-body Q-box to 2nd order

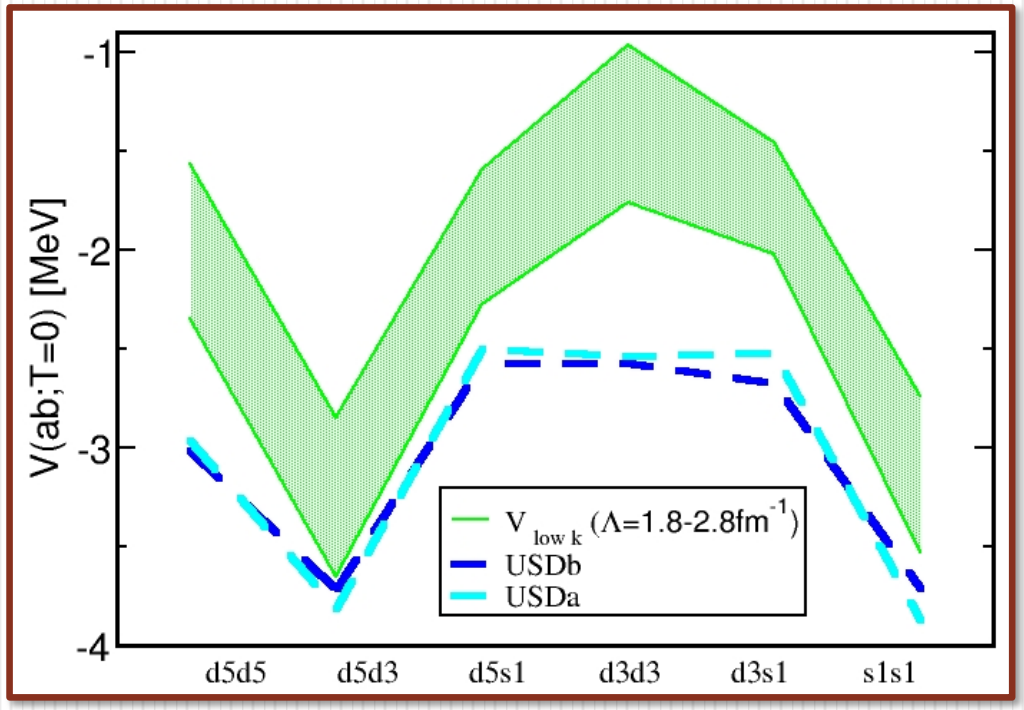
- Effective interaction given by folded diagram expansion:

$$V_{\text{eff}} = \hat{Q} - \hat{Q}' \int \hat{Q} + \hat{Q}' \int \hat{Q} \int \hat{Q} - \hat{Q}' \int \hat{Q} \int \hat{Q} \int \hat{Q} + \ldots$$

- **Single-particle energies** can be calculated…
  - Traditionally taken from experimental one-particle spectrum or empirical values

Cutoff Dependence of Monopoles

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



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Microscopic Approach: Chiral EFT

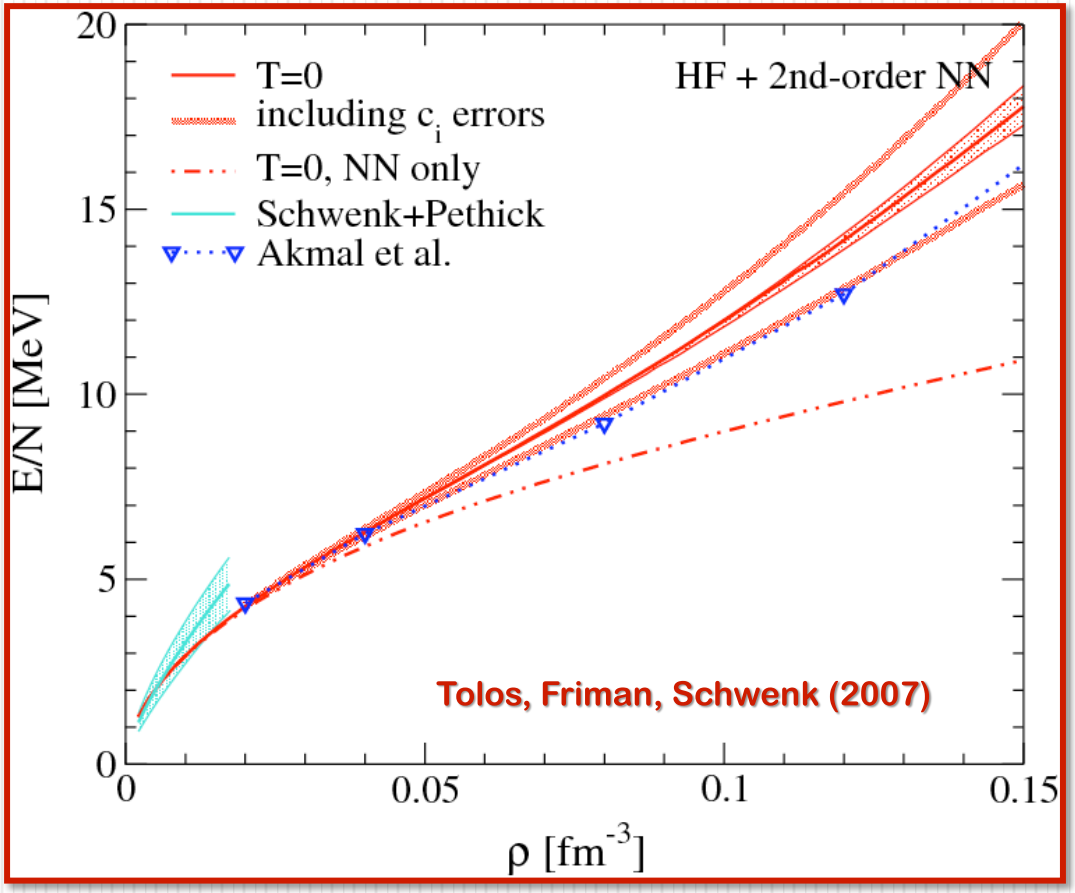
- Examine low-energy chiral properties of QCD using EFT
- In most nuclei $Q \sim m_\pi$, so π exchange must be included
- Nucleons and pions explicit degrees of freedom
- Nucleons interact via π exchange and contact interactions
- Theory can be organized in powers of $\left(\frac{Q}{\Lambda_\chi}\right)$, valid for low-mom.
- Irreducible time-ordered diagram has order: $\left(\frac{Q}{\Lambda_\chi}\right)^\nu$, $\Lambda_\chi \approx 700\,\mathrm{MeV}$

$$\nu = -2 + 2N + 2(L - C) + \sum_i V_i \Delta_i$$

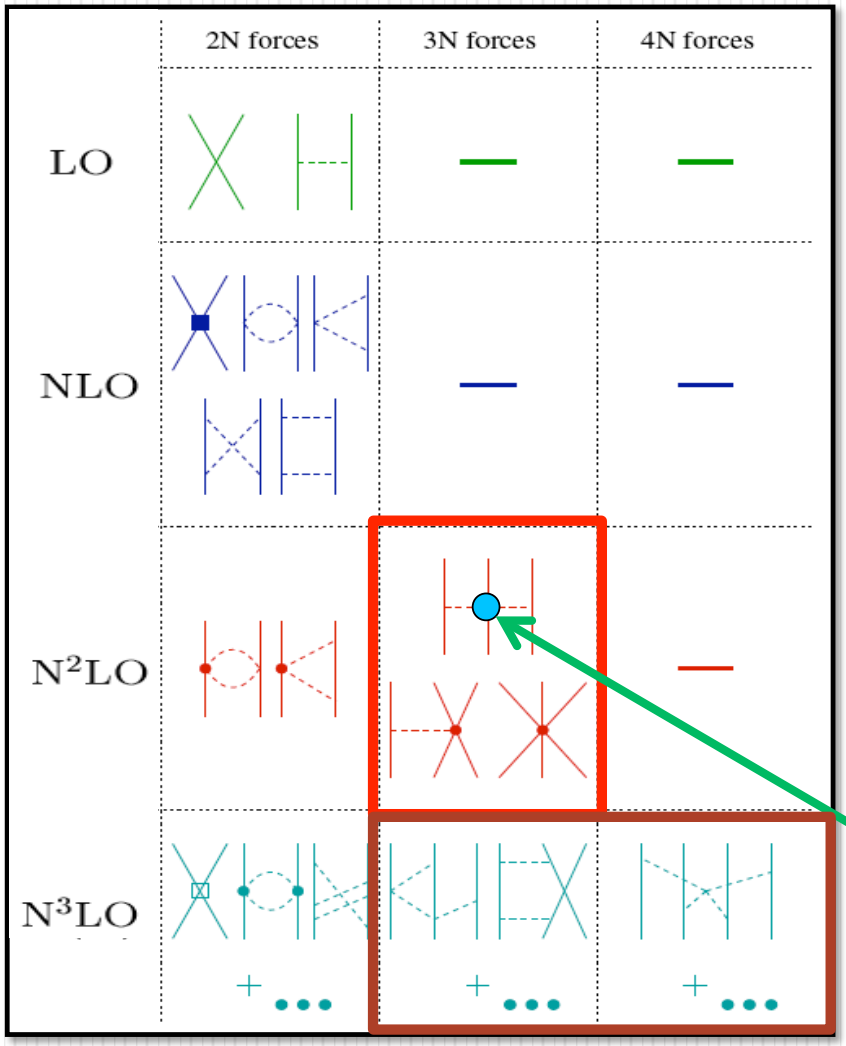
$\Delta_i = d_i + \frac{1}{2} n_i - 2$ "Chiral dimension" of vertex

Uncertainty in c-terms

- In neutron matter, large uncertainty in c-terms dominates variation in cutoff



Chiral EFT: Summary



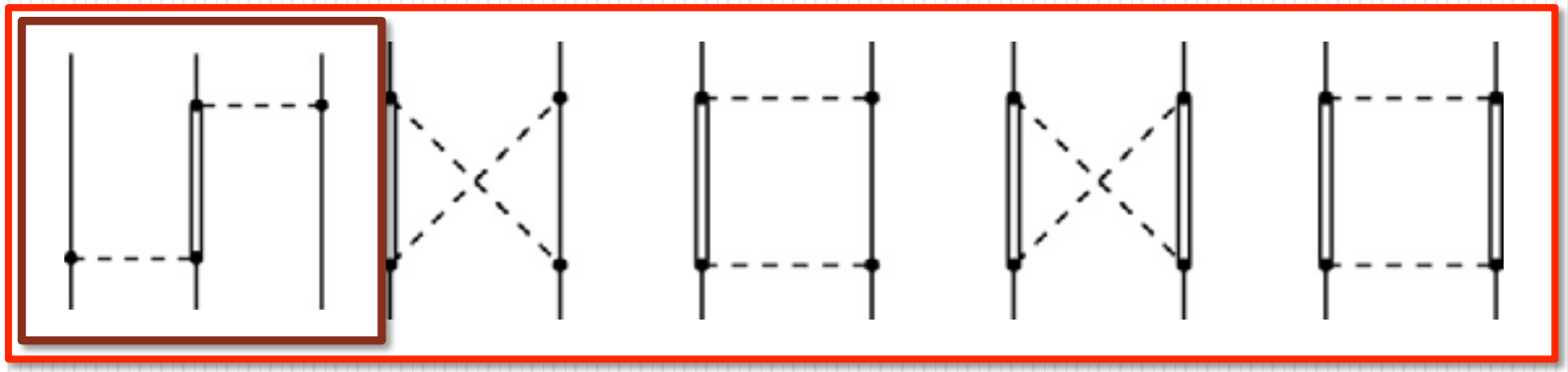
- Nucleons interact via π exchange and contact interactions
- Explains hierarchy: $V_{\mathrm{NN}} > V_{\mathrm{3N}} > \ldots$
- Short-range couplings fit to experiment
- Systematic way to include 3NF with low-momentum interactions
- Only two new couplings at N²LO:
  c terms: already constrained by NN, πN data

$$c_1 = -0.9^{+0.2}_{-0.5},\ c_3 = -4.7^{+1.2}_{-1.0}$$
$$c_4 = 3.5^{+0.5}_{-0.2}$$

- None at N³LO for 3N, 4N!

Intermediate Δ-Excitations

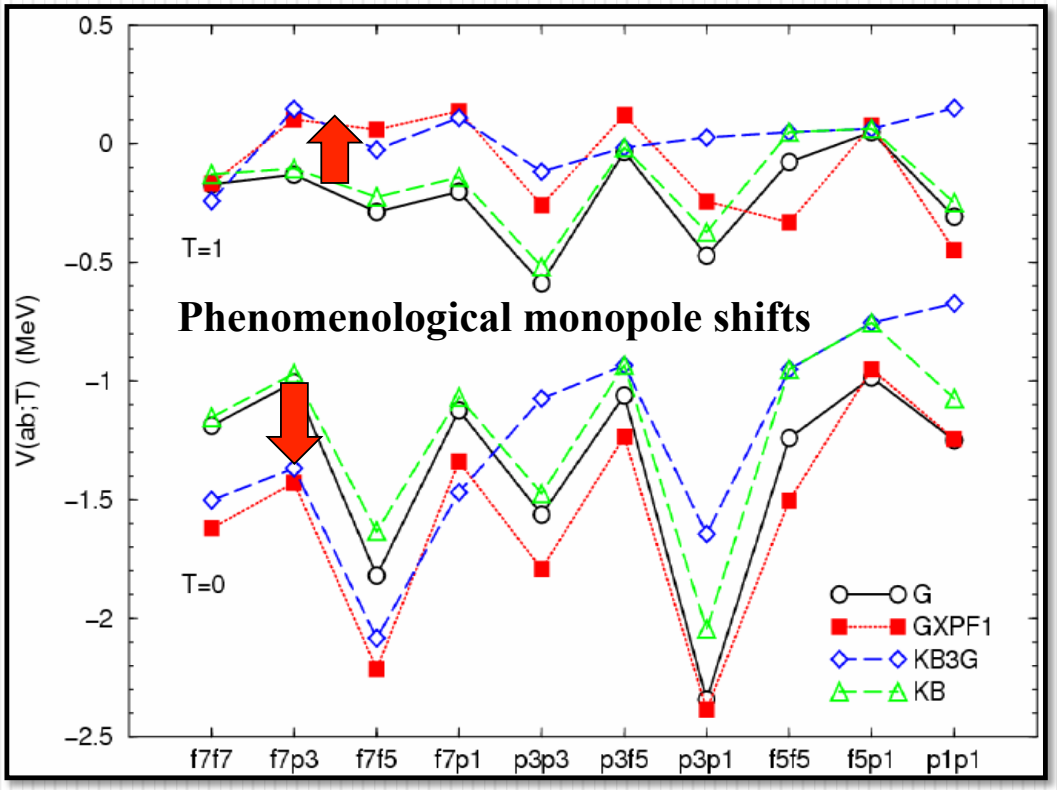
- Importance of Δ-isobar is well known:
  - Small excitation energy: $\Delta m = 293\ \mathrm{MeV}$
  - Strong coupling to πN system
- Can be included explicitly in chiral EFT
- Leading contributions enter at NLO, 3N at N²LO



- 2π-exchange diagram has structure analogous to corresponding chiral EFT diagram with:

$$c_1 = 0, c_3 = -2c_4 = \frac{h_A^2}{9\Delta m}; h_A = \frac{3g_A}{\sqrt{2}}$$

Phenomenological vs. Microscopic

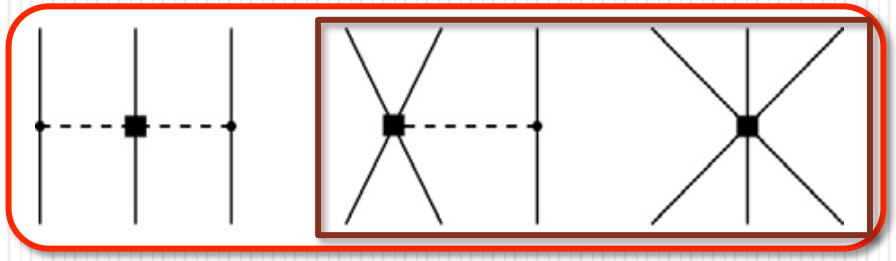


Compare monopoles from:

- *Microscopic* **G-matrix**, **Kuo-Brown** interactions
- *Phenomenological* **GXPF1**, **KB3G** interactions.
  Clear shifts for *low-lying orbitals*:
  - T=1 repulsive shift
  - T=0 attractive shift

van Kolck (1994), Epelbaum et al. (2002)

Chiral EFT: 3N Forces



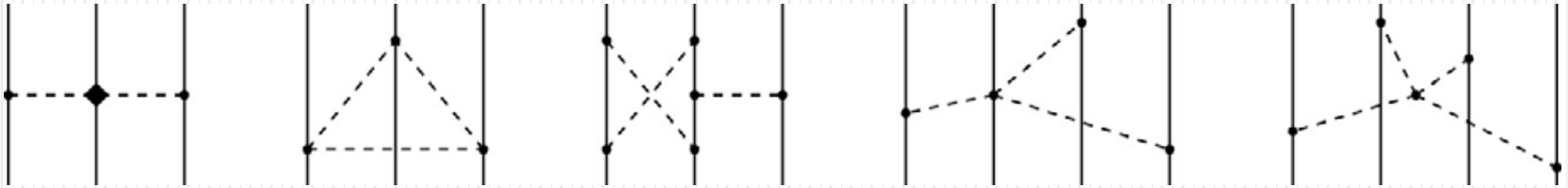
- 2 new couplings: D, E

- Intermediate range OPE interaction:

$$V^{(3)}_{1\pi,\,\mathrm{cont}} = -\sum_{i\neq j\neq k}\left(\frac{g_A}{8F_\pi}\right)^2 D\,\frac{(\vec{\sigma}_j\cdot\vec{q}_j)}{(\vec{q}_j^{\,2}+M_\pi^2)}(\tau_i\cdot\tau_j)(\vec{\sigma}_i\cdot\vec{\sigma}_j)$$

- Short range contact interaction: $V^{(3)}_{\mathrm{cont}} = \frac{1}{2}\sum_{j\neq k} E(\tau_j\cdot\tau_k)$

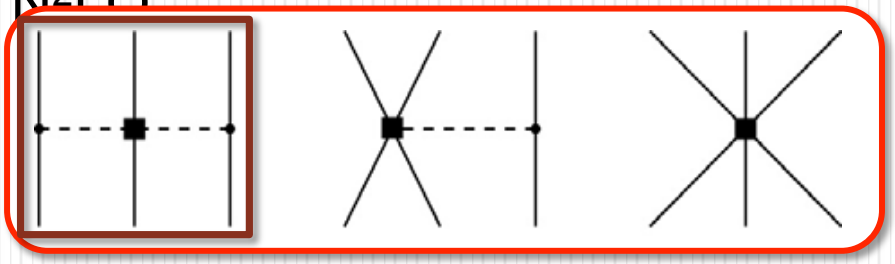
- 3NF at N^{3}LO and 4NF in progress:



van Kolck (1994), Epelbaum et al. (2002)

Chiral EFT: 3N Forces

- 3N forces arise naturally – first non-vanishing at order $\nu = 3$ N2LO



- First look at 2π-exchange long range interaction

$$V_{2\pi}^{(3)} = \sum_{i\neq j\neq k} \frac{1}{2}\left(\frac{g_A}{2F_\pi}\right)^2 \frac{(\vec{\sigma}_i\cdot\vec{q}_i)(\vec{\sigma}_j\cdot\vec{q}_j)}{(\vec{q}_i^{\,2}+M_\pi^2)(\vec{q}_j^{\,2}+M_\pi^2)} F_{ijk}^{\alpha\beta}\tau_i^\alpha\tau_j^\beta$$

$$F_{ijk}^{\alpha\beta} = \delta^{\alpha\beta}\left(-\frac{4c_1M_\pi^2}{F_\pi^2}+\frac{2c_3}{F_\pi^2}\vec{q}_i\cdot\vec{q}_j\right)+\sum_\gamma\frac{c_4}{F_\pi^2}\varepsilon^{\alpha\beta\gamma}\tau_k^\gamma\vec{\sigma}_k\cdot(\vec{q}_i\times\vec{q}_j)$$

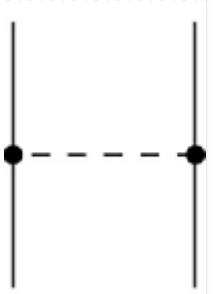
- 3 LECs: c_1, c_3, c_4 – already determined from 2N chiral int.

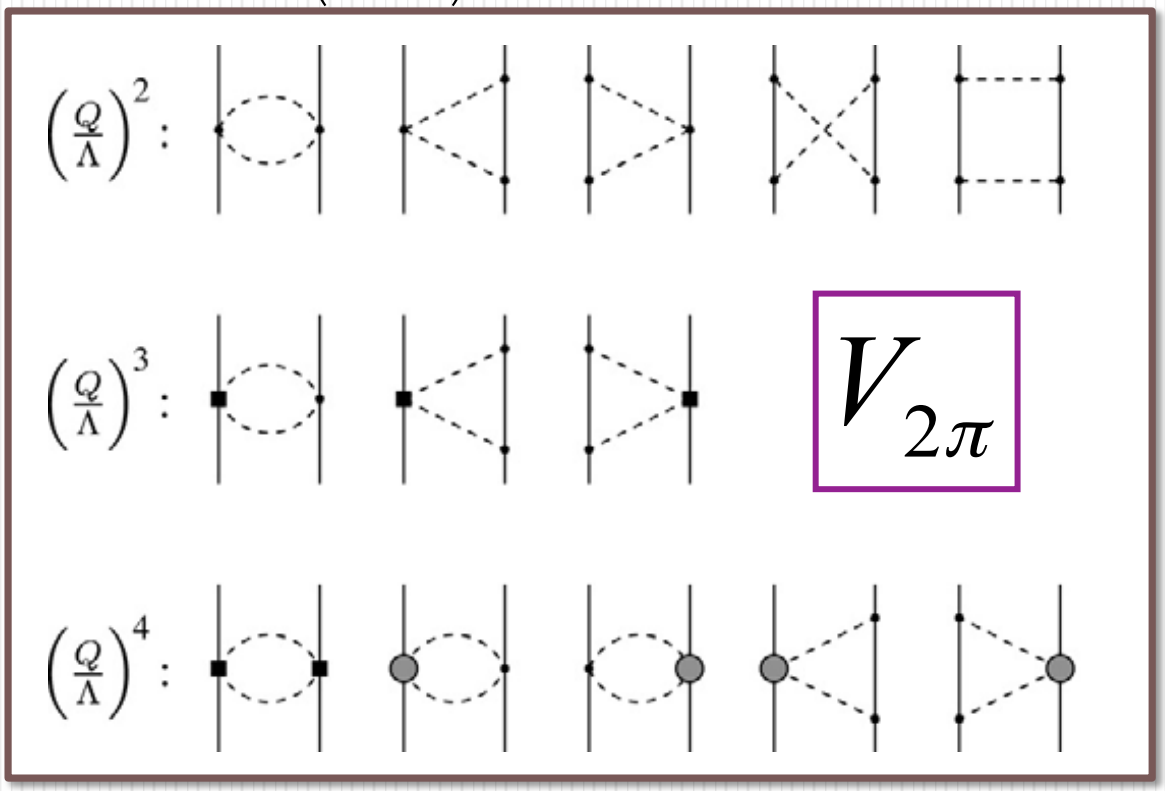
Van Kolck (1994), Epelbaum et al. (2002)

Chiral EFT: 2N Forces

$$V_{2N} = V_\pi + V_{\text{cont}} \qquad V_\pi = V_{1\pi} + V_{2\pi} + V_{3\pi} + \cdots$$

$$V_{1\pi} = -\left(\frac{g_A}{2F_\pi}\right)^2 \frac{(\vec{\sigma}_1 \cdot \vec{q})(\vec{\sigma}_2 \cdot \vec{q})}{(\vec{q}^{\,2} + M_\pi^2)} \tau_1 \tau_2$$





$$\vec{q}_i \equiv \vec{p}\,'_i - \vec{p}_i$$

$$g_A = 1.26$$

$$F_\pi = 92.4\ \text{MeV}$$

- Coupling constants: c_i fit to πN, NN scattering data