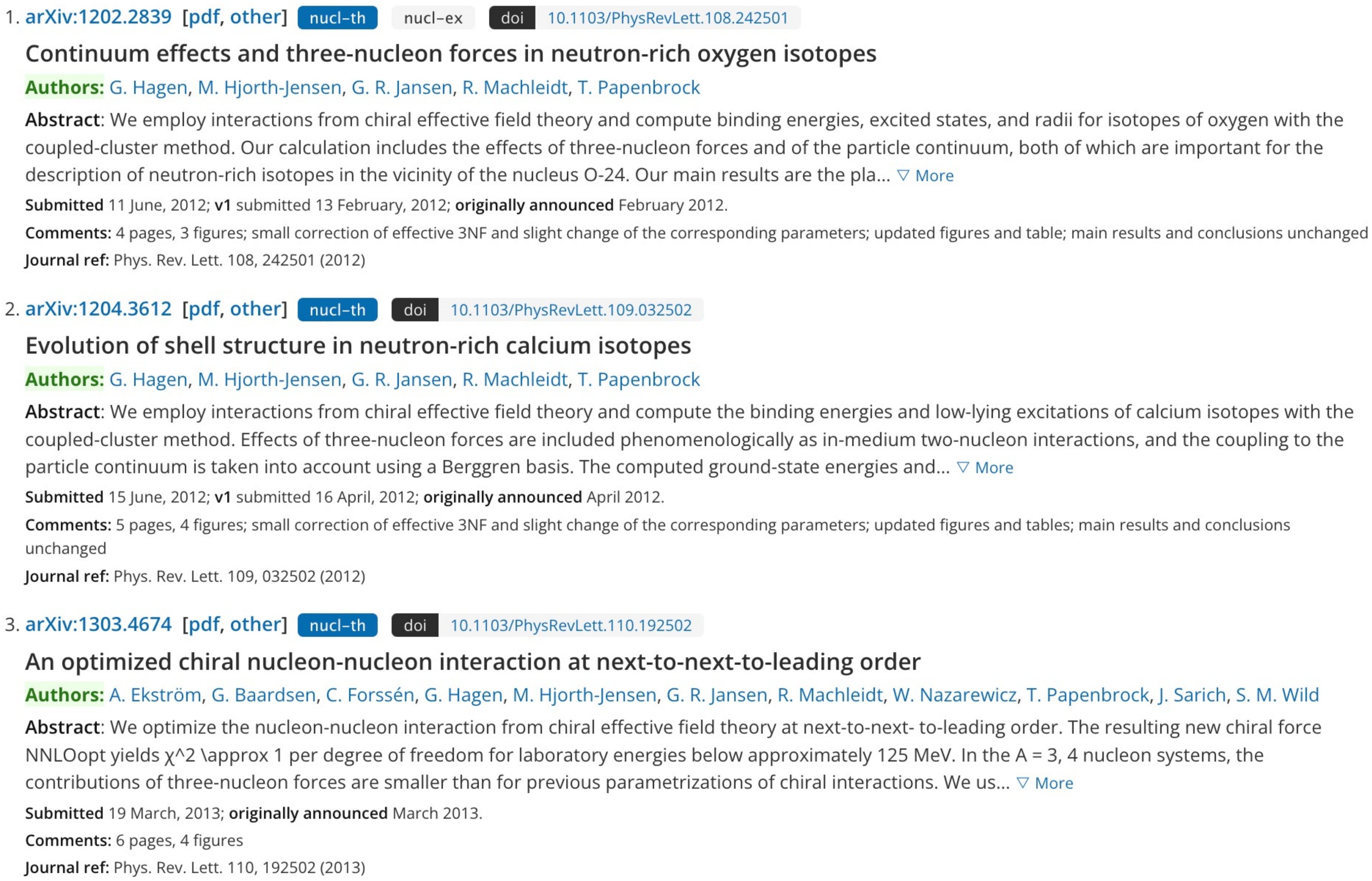
Ruprecht Machleidt



1. arXiv:1202.2839 [pdf, other] nucl-th nucl-ex doi 10.1103/PhysRevLett.108.242501

Continuum effects and three-nucleon forces in neutron-rich oxygen isotopes

Authors: G. Hagen, M. Hjorth-Jensen, G. R. Jansen, R. Machleidt, T. Papenbrock

Abstract: We employ interactions from chiral effective field theory and compute binding energies, excited states, and radii for isotopes of oxygen with the coupled-cluster method. Our calculation includes the effects of three-nucleon forces and of the particle continuum, both of which are important for the description of neutron-rich isotopes in the vicinity of the nucleus O-24. Our main results are the pla… ▽ More

Submitted 11 June, 2012; **v1** submitted 13 February, 2012; **originally announced** February 2012.

Comments: 4 pages, 3 figures; small correction of effective 3NF and slight change of the corresponding parameters; updated figures and table; main results and conclusions unchanged

Journal ref: Phys. Rev. Lett. 108, 242501 (2012)

2. arXiv:1204.3612 [pdf, other] nucl-th doi 10.1103/PhysRevLett.109.032502

Evolution of shell structure in neutron-rich calcium isotopes

Authors: G. Hagen, M. Hjorth-Jensen, G. R. Jansen, R. Machleidt, T. Papenbrock

Abstract: We employ interactions from chiral effective field theory and compute the binding energies and low-lying excitations of calcium isotopes with the coupled-cluster method. Effects of three-nucleon forces are included phenomenologically as in-medium two-nucleon interactions, and the coupling to the particle continuum is taken into account using a Berggren basis. The computed ground-state energies and… ▽ More

Submitted 15 June, 2012; **v1** submitted 16 April, 2012; **originally announced** April 2012.

Comments: 5 pages, 4 figures; small correction of effective 3NF and slight change of the corresponding parameters; updated figures and tables; main results and conclusions unchanged

Journal ref: Phys. Rev. Lett. 109, 032502 (2012)

3. arXiv:1303.4674 [pdf, other] nucl-th doi 10.1103/PhysRevLett.110.192502

An optimized chiral nucleon-nucleon interaction at next-to-next-to-leading order

Authors: A. Ekström, G. Baardsen, C. Forssén, G. Hagen, M. Hjorth-Jensen, G. R. Jansen, R. Machleidt, W. Nazarewicz, T. Papenbrock, J. Sarich, S. M. Wild

Abstract: We optimize the nucleon-nucleon interaction from chiral effective field theory at next-to-next- to-leading order. The resulting new chiral force NNLOopt yields χ^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 us… ▽ More

Submitted 19 March, 2013; **originally announced** March 2013.

Comments: 6 pages, 4 figures

Journal ref: Phys. Rev. Lett. 110, 192502 (2013)

Error to report

- Our coupled-cluster computations with 3NFs in nuclear matter were wrong.
- Impact:
    - $\mathrm{NNLO}_{\mathrm{sat}}$ has more accurate nuclear matter properties than previously reported
    - $\Delta\mathrm{NNLO}_{\mathrm{GO}}$ (which was fit to nuclear matter saturation) is overbound and saturates at too high density
- Errata have been published / are being prepared

Thanks to Weiguang Jiang, Francesco Marino , and Sam Novario for identifying this problem.

The magnetic dipole transition in ^{48}Ca – a mystery

Thomas Papenbrock

University of Tennessee & Oak Ridge National Laboratory

TRIUMF workshop on *Progress in Ab Initio Nuclear Theory*, 2/28/2024

SciDAC
Scientific Discovery through Advanced Computing

Work supported by the US Department of Energy

NUCLEI
Nuclear Computational Low-Energy Initiative
A SciDAC-5 collaboration

Collaborators

Bijaya Acharya, Baishan Hu, Gaute Hagen (ORNL)

Sonia Bacca (Mainz)

Petr Navratil (TRIUMF)

Bijaya Acharya, Baishan Hu, S. Bacca, G. Hagen, P. Navratil, TP,
“The magnetic dipole transition in ^{48}Ca,” arXiv:2311.11438

Why do people care about M1 transitions?

Supernova 1987A

February 24, 1987
Las Campanas Observatory

M1 spin excitations are dominated by isovector contributions.

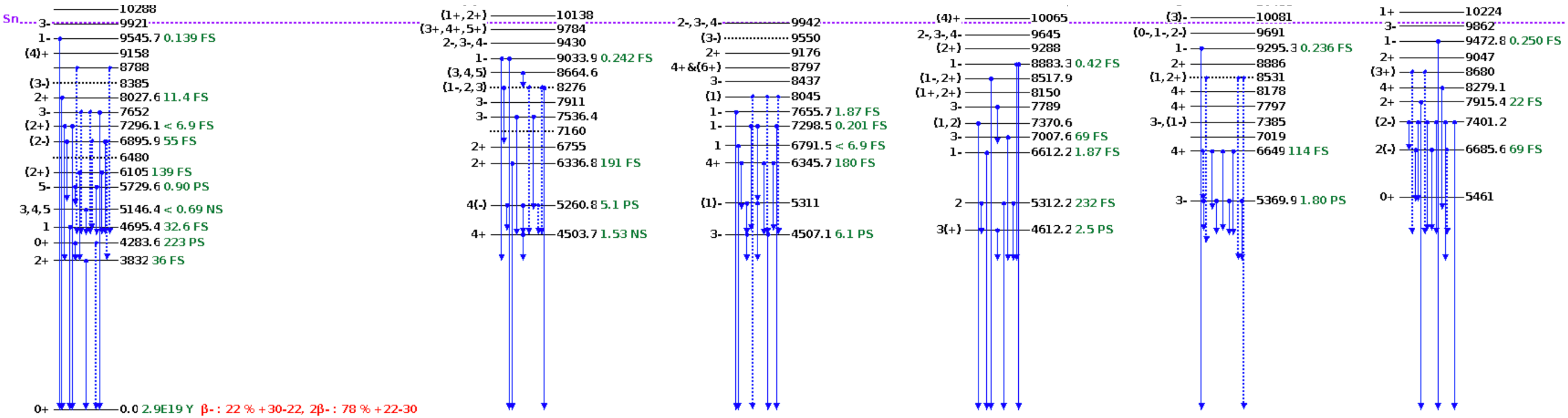
The isovector-0 component of the Gamow-Teller operator translates to inelastic neutral-current neutrino-nucleus reactions at energies relevant for supernovae.

Our understanding of M1 impacts supernovae signals and dynamics.

Lüttge, von Neumann-Cosel, Neumeyer, Richter, Nucl Phys A (1996);
Langanke, Martinez-Pinedo, von Neumann-Cosel, Richter, Phys Rev Lett (2004);
Loens, Langanke, Martinez-Pinedo, Sieja, EPJA (2012);
Tornow et al, Phys Letts B (2022).

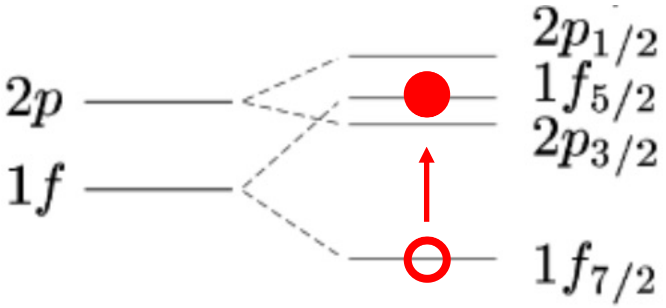
Review on $M1$:
K. Heyde, P. von Neumann-Cosel, A. Richter, Rev. Mod. Phys. 82, 2365 (2010).

The resonant 1^+ state in ^{48}Ca at 10.224 MeV

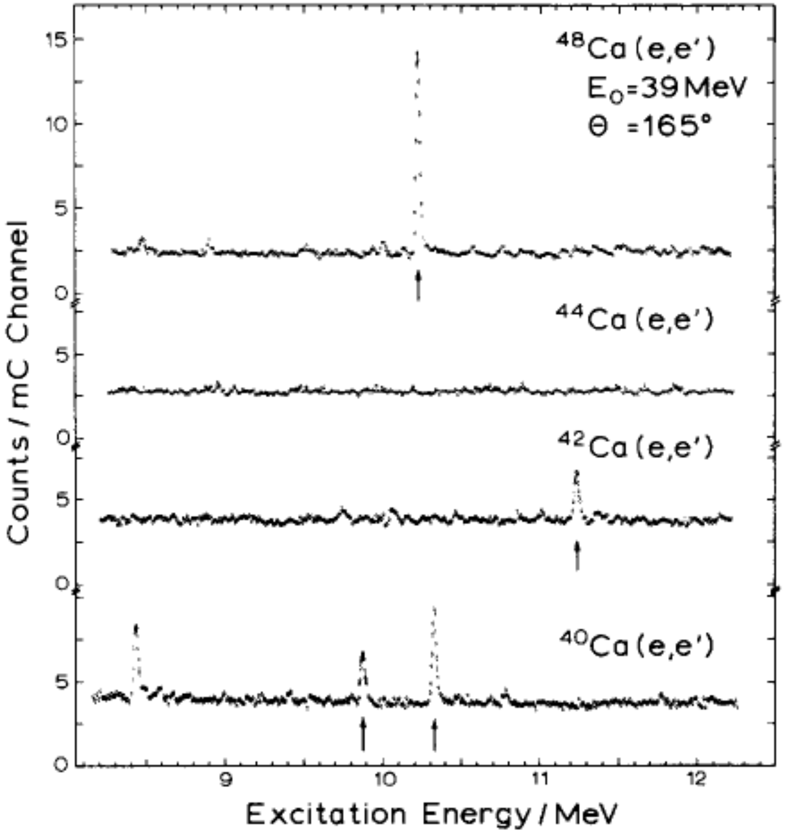


Scattering / reactions that probe the 1^+ state: (e,e'), (p,p'), (p,n), or (γ,n)

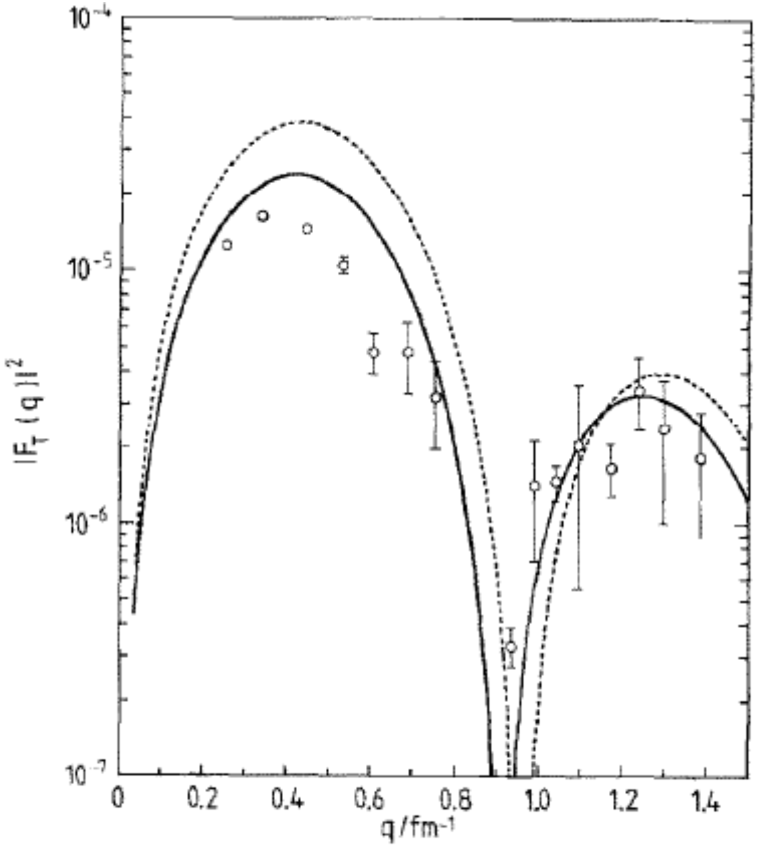
Simple picture of the 1^+ state: neutron 1p-1h excitation; extreme single-particle model: $B(M1) = 12\ \mu_N^2$



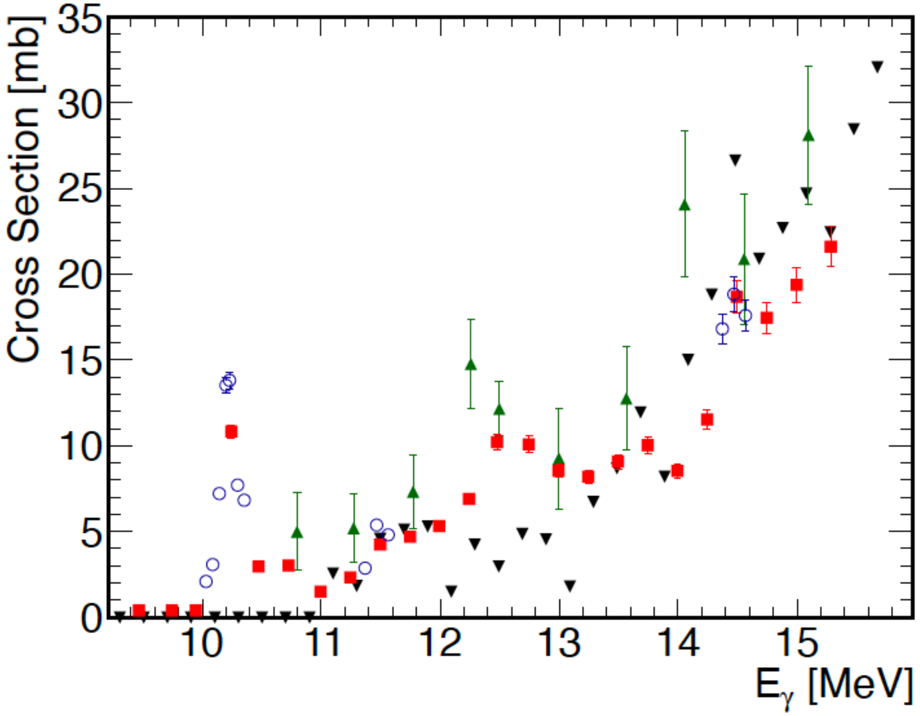
The mystery



Steffen et al., Phys. Letts. B (1980)
(e, e') scattering sees a peak, interpreted as M1 resonance



Steffen et al., Nucl. Phys. A (1983)
form factor compared to shell model and quenched shell model
$B(M1) = 4.0 \pm 0.3\ \mu_N^2$



Tompkins et al, Phys Rev C (2011)
$^{48}Ca(\gamma, n)$ experiment yields
$B(M1) = 6.8 \pm 0.5\ \mu_N^2$

?!

The plot thickens

(e, e') scattering: $B(M1) = 4.0 \pm 0.3\ \mu_N^2$ [Steffen et al 1980; 1983]
(γ, n) scattering: $B(M1) = 6.8 \pm 0.5\ \mu_N^2$ [Tompkin et al 2011]
(p, p') scattering: $B(M1) = 3.85(32) - 4.63(38)\ \mu_N^2$ [Birkhan et al 2016]

Extreme s.p. model: $B(M1) = 12\ \mu_N^2$

Theory has a hard time to reproduce a large amount of quenching

A. Harting, W. Weise, H. Toki, and A. Richter, Physics Letters B 104, 261 (1981).

} Meson-exchange currents explain small $B(M1)$

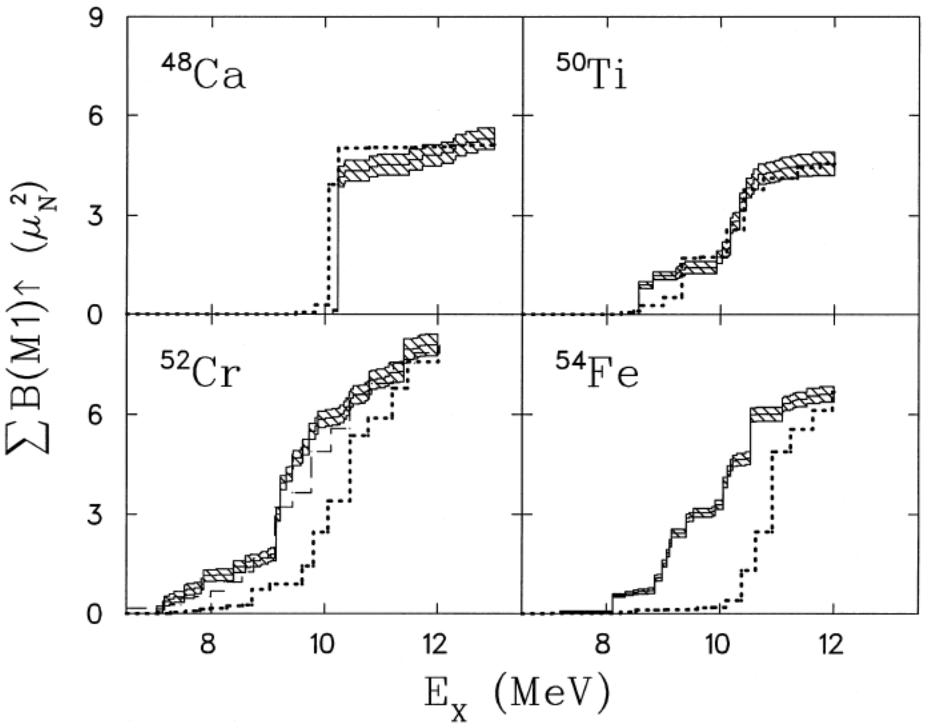
J. B. McGrory and B. H. Wildenthal, Phys. Lett. B 103, 173 (1981).
Toru Suzuki, S. Krewald, and J. Speth, Physics Letters B 107, 9 (1981).
G. F. Bertsch, Nuclear Physics A 354, 157 (1981).
M. Kohno and D. W. L. Sprung, Phys. Rev. C 26, 297 (1982).
K. Takayanagi, K. Shimizu, and A. Arima, Nuclear Physics A 481, 313 (1988).
M. G. E. Brand, K. Allaart, and W. H. Dickhoff, Nuclear Physics A 509, 1 (1990).
B. A. Brown and W. A. Richter, Phys. Rev. C 58, 2099 (1998).

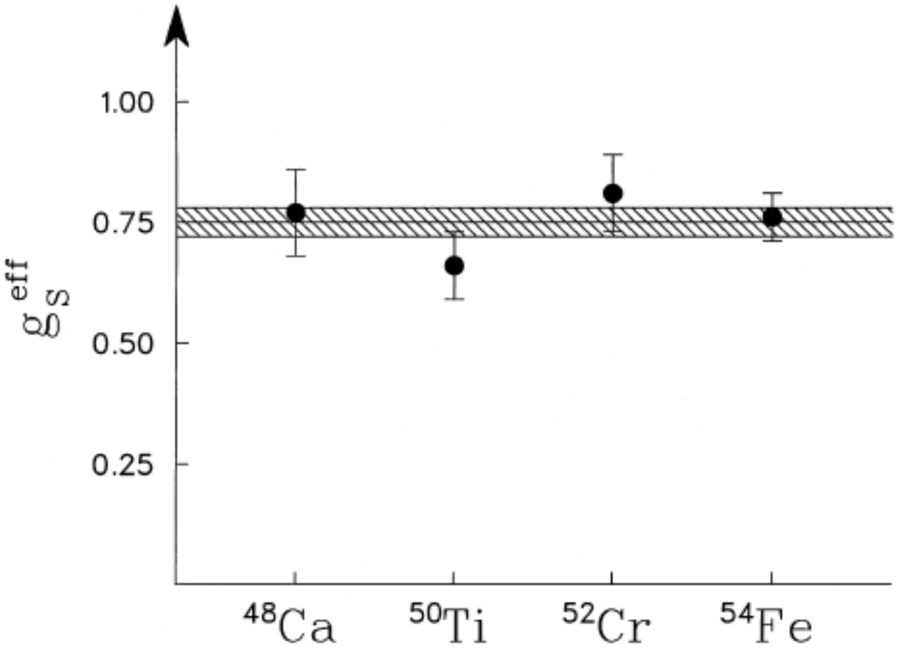
} All too high $B(M1)$;
$B(M1) = 7 - 8\mu_N^2$;
$B(M1) > 5.1\mu_N^2$;

J. D. Holt, J. Menendez, J. Simonis, and A. Schwenk, Phys. Rev. C 90, 024312 (2014).
J. Wilhelmy, et al., Phys. Rev. C 98, 034315 (2018).

} Reproduce (e, e') $B(M1)$ if quenched

Why could/should there be quenching?





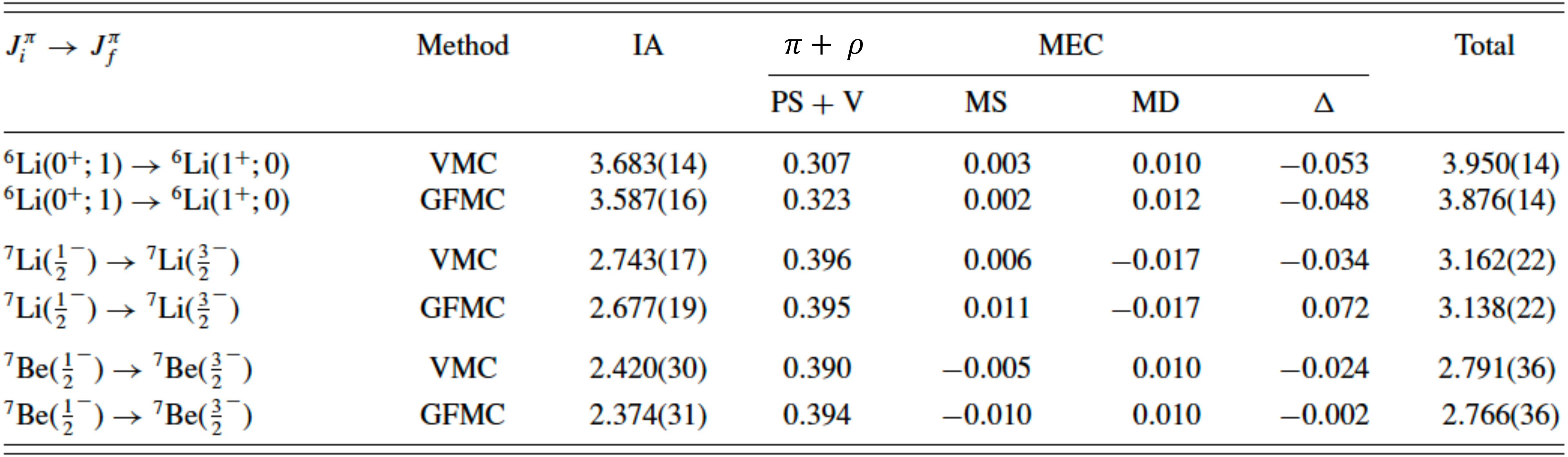
Results from (e, e') scattering match quenched shell-model results

Von Neumann-Cosel, Poves, Retamosa, Richter, Phys Letts B (1998)

Proposed: $B(M1)$ is quenched similarly to $B(GT)$ in pf shell nuclei

→ Impacts (re)analyses of (p, p') experiments using the “unit cross section” method

Two-body currents do not quench M1 transitions in light nuclei



$J_i^\pi \to J_f^\pi$	Method	IA	$\pi + \rho$ MEC				Total
			PS + V	MS	MD	Δ	
^{6}Li$(0^+;1) \to {}^6$Li$(1^+;0)$	VMC	3.683(14)	0.307	0.003	0.010	−0.053	3.950(14)
^{6}Li$(0^+;1) \to {}^6$Li$(1^+;0)$	GFMC	3.587(16)	0.323	0.002	0.012	−0.048	3.876(14)
^{7}Li$(\frac{1}{2}^-) \to {}^7$Li$(\frac{3}{2}^-)$	VMC	2.743(17)	0.396	0.006	−0.017	−0.034	3.162(22)
^{7}Li$(\frac{1}{2}^-) \to {}^7$Li$(\frac{3}{2}^-)$	GFMC	2.677(19)	0.395	0.011	−0.017	0.072	3.138(22)
^{7}Be$(\frac{1}{2}^-) \to {}^7$Be$(\frac{3}{2}^-)$	VMC	2.420(30)	0.390	−0.005	0.010	−0.024	2.791(36)
^{7}Be$(\frac{1}{2}^-) \to {}^7$Be$(\frac{3}{2}^-)$	GFMC	2.374(31)	0.394	−0.010	0.010	−0.002	2.766(36)

Marcucci, Muslema Pervin, Pieper, Schiavilla, Wiringa, Phys Rev C 78, 065501 (2008)

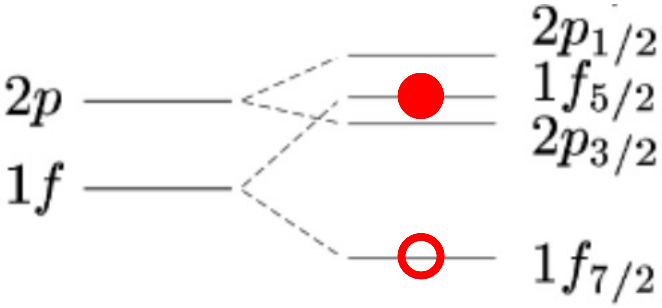
This is similar to what we will use

This is perhaps similar to what people used in the 1980s

Two-body currents for $M1$ transitions differ from those for Gamow-Teller transitions

An interesting and challenging problem…
…for *Ab Initio*

Conceptually simple:
neutron 1p-1h excitation
$\left(a^{+}_{5/2} \times a_{7/2}\right)^{(1)} |^{48}Ca\rangle$



→ Coupled-cluster method seems attractive for this

However: The excited 1^{+} state at $E_{1^{+}} = 10.224$ MeV is just above the threshold for neutron emission, and we have $S_n = 9.952$ MeV

(It seems all previous computations considered only bound states)

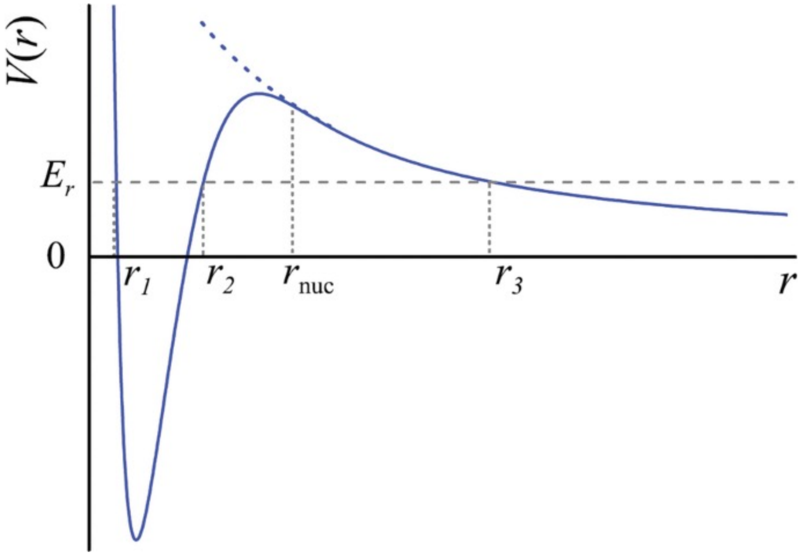
→ Need to use Gamow basis that includes resonances and continuum effects

…and: (e, e') and (p, p') experiments indicated that a lot of quenching is going on.

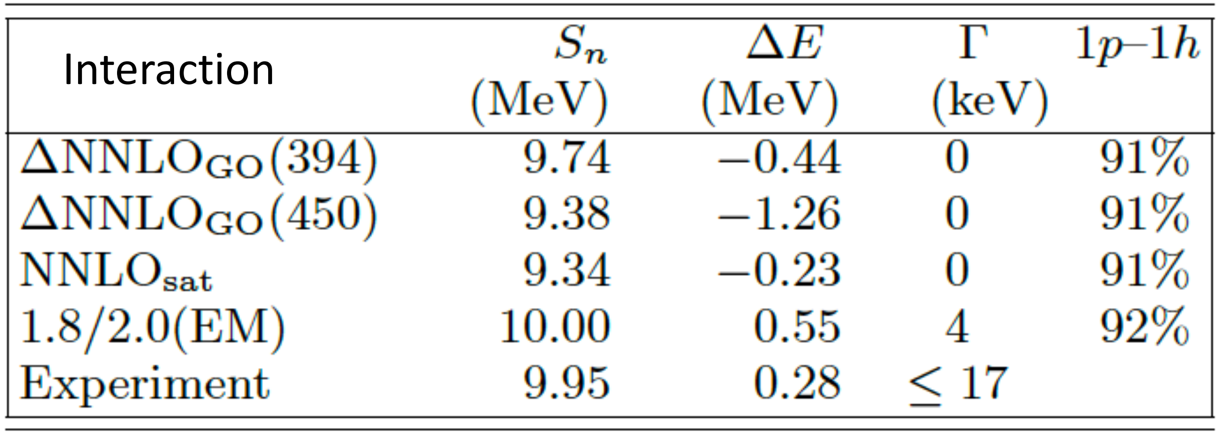
Where does this come from?

→ Need to include two-body currents

The resonant 1^+ state in ^{48}Ca at 10.224 MeV



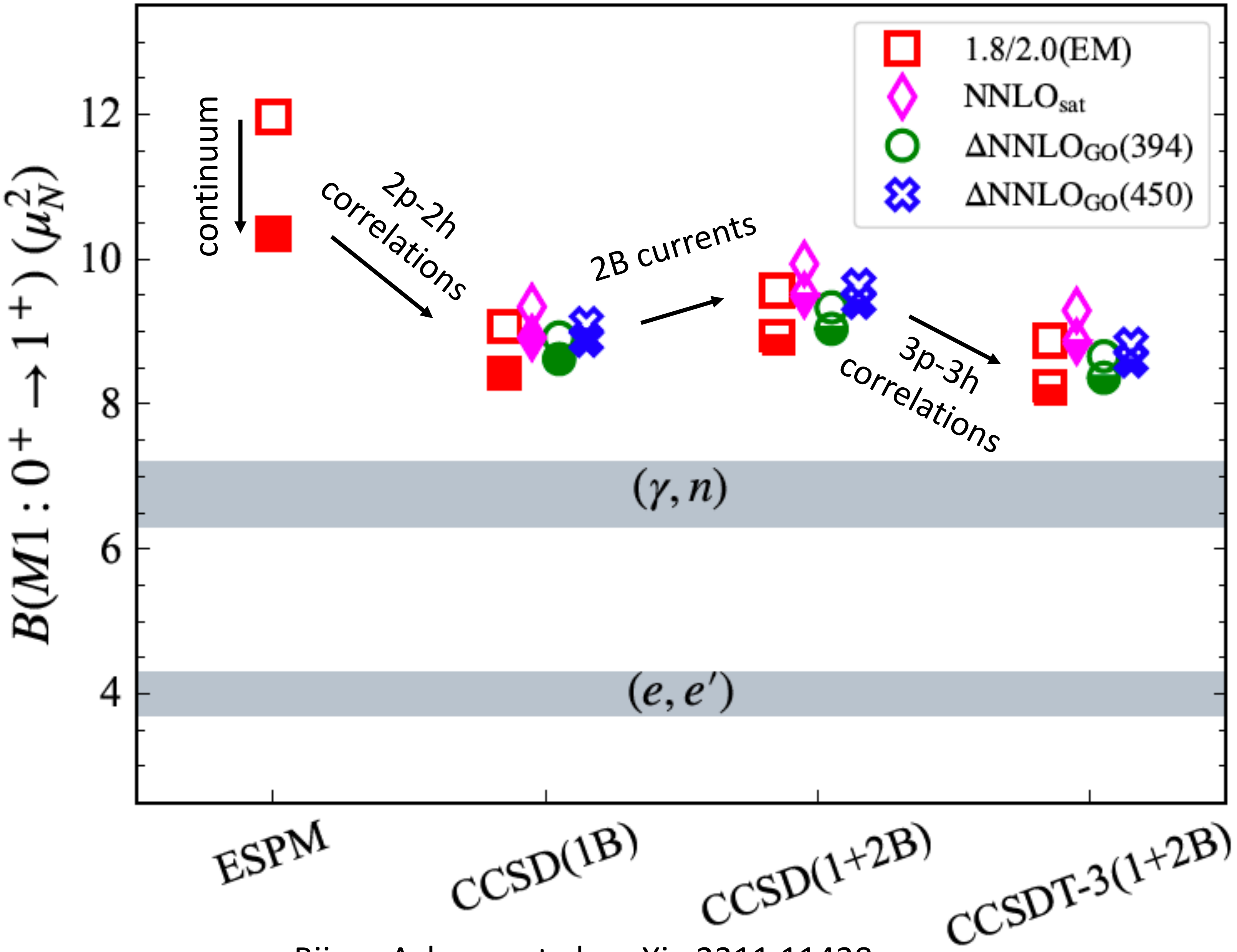
The $l = 3$ orbital angular-momentum barrier permits a neutron resonant state



Interaction	S_n (MeV)	ΔE (MeV)	Γ (keV)	$1p$–$1h$
ΔNNLO$_{\mathrm{GO}}$(394)	9.74	−0.44	0	91%
ΔNNLO$_{\mathrm{GO}}$(450)	9.38	−1.26	0	91%
NNLO$_{\mathrm{sat}}$	9.34	−0.23	0	91%
1.8/2.0(EM)	10.00	0.55	4	92%
Experiment	9.95	0.28	≤ 17	

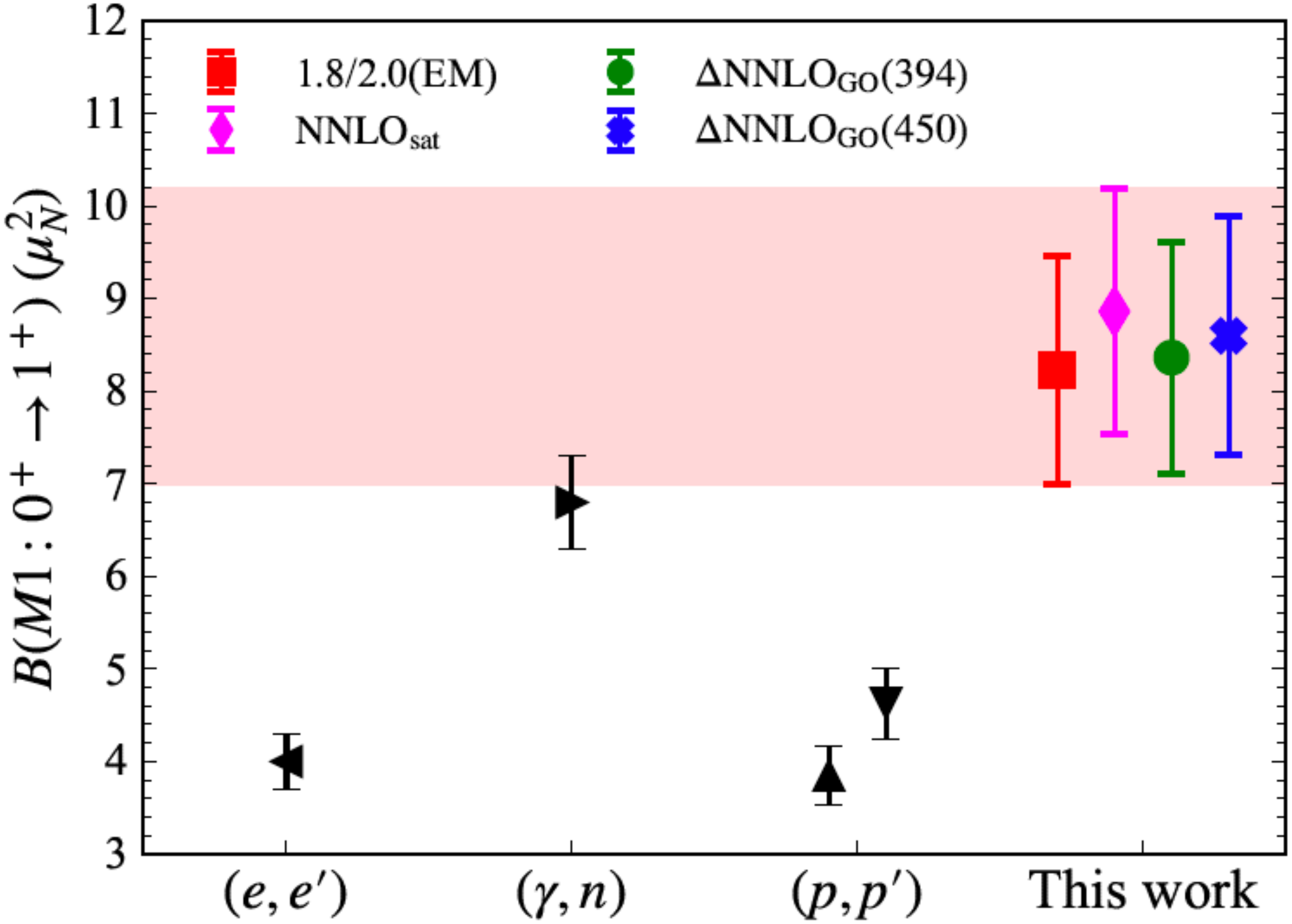
Bijaya Acharya et al., arXiv:2311.11438

Contributions to $B(M1)$



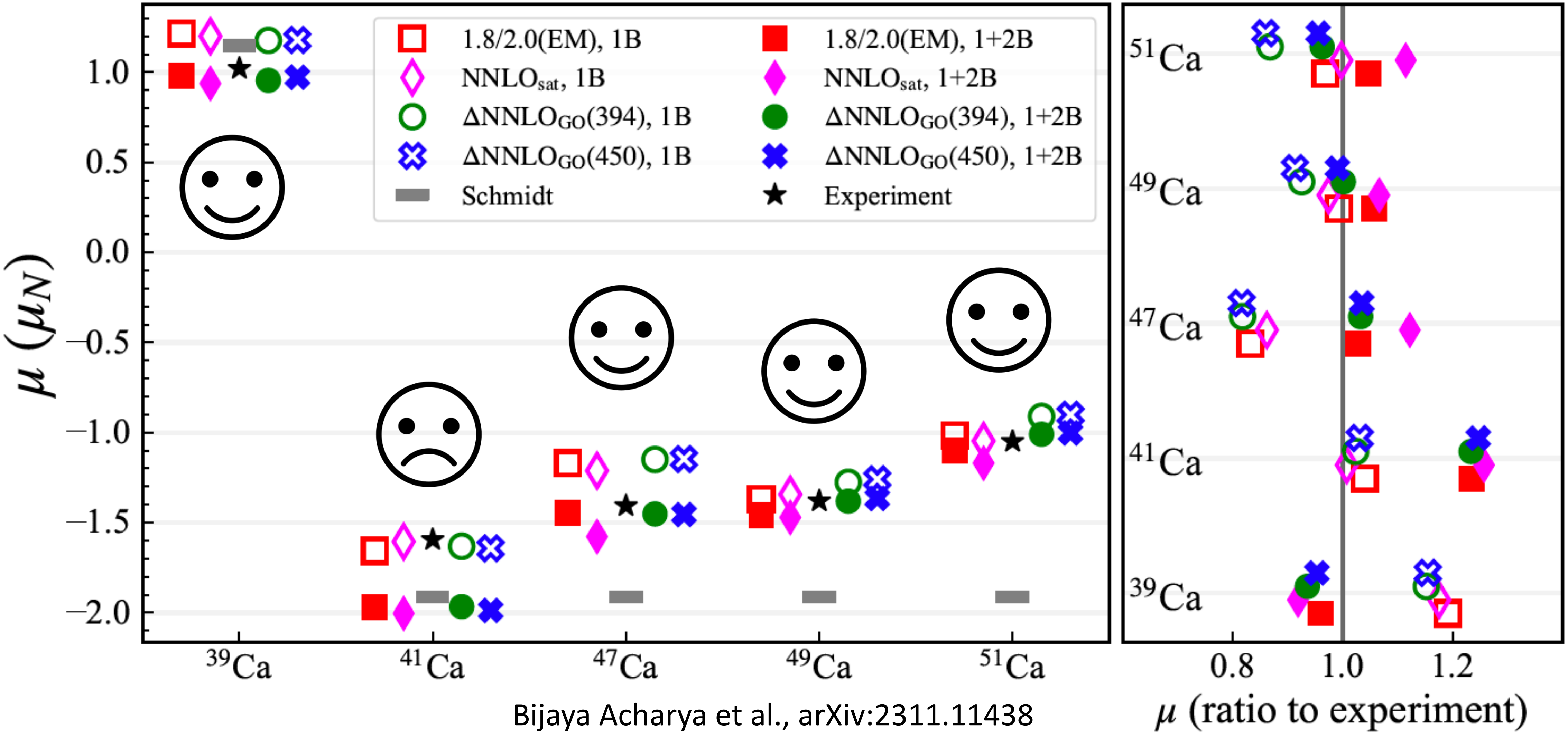
Bijaya Acharya et al., arXiv:2311.11438

Final result



Bijaya Acharya et al., arXiv:2311.11438

Magnetic moments



Bijaya Acharya et al., arXiv:2311.11438

Takayuki Miyagi et al., arXiv:2311.14383, propose that multi-shell VS-IMSRG calculation yields accurate results for ^{41}Ca.

Almost Summary

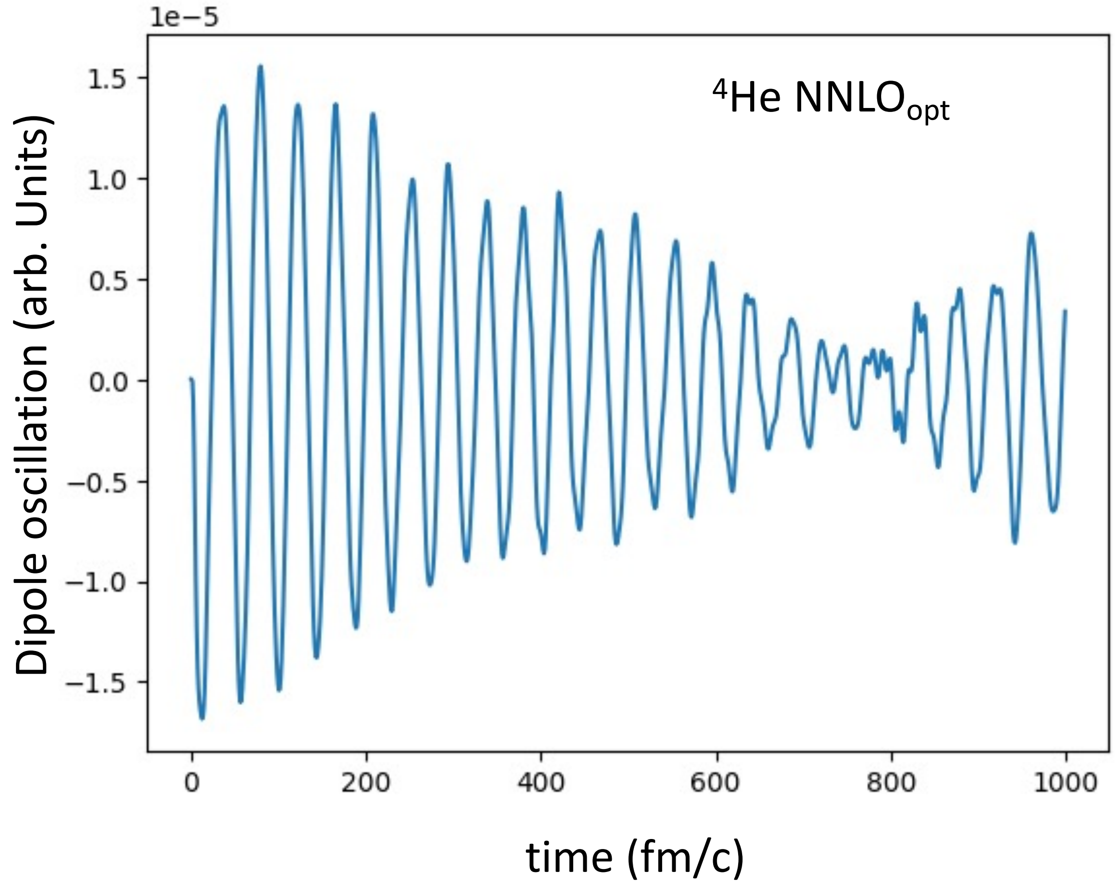
- The discrepancy between (e, e') and (γ, n) experiments regarding $B(M1)$ in ^{48}Ca is puzzling
- Our ab initio computations based on chiral effective field theory, including treatment of the state as a resonance, yield $7\mu_N^2 < B(M1) < 10\ \mu_N^2$
  - Two-body currents do not yield quenching of $B(M1)$
  - Similar to what was found in light nuclei
- Resolution of this puzzle will impact ab initio computations and/or theory of neutrino-nucleus reactions relevant for supernova signals and dynamics

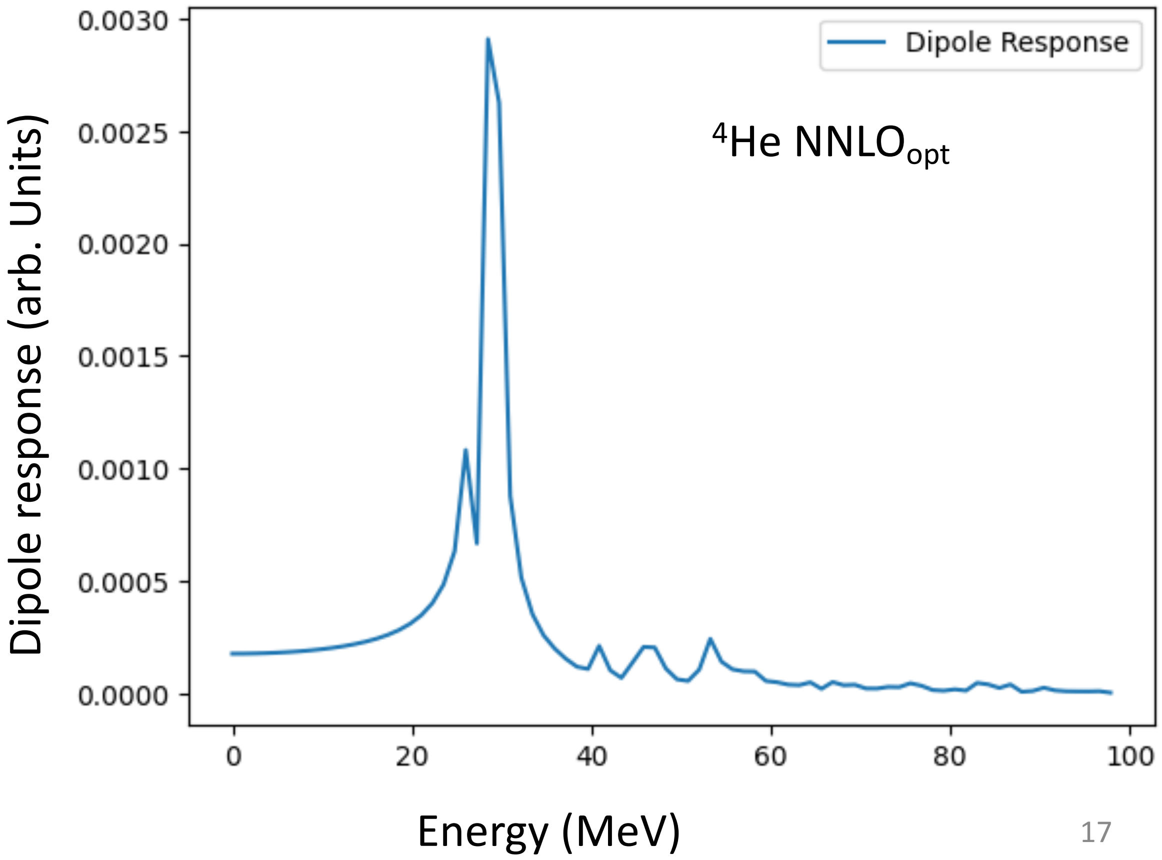
Time-dependent coupled-cluster method

Dusted off (and updated!) time-dependent coupled cluster code [Pigg, Hagen, Nam, TP, Phys Rev C 2012].

$$\overline{H}|\Phi\rangle = i\hbar e^{-S}\partial_t e^{S}|\Phi\rangle \qquad \overline{H} \equiv e^{-S} H e^{S}$$

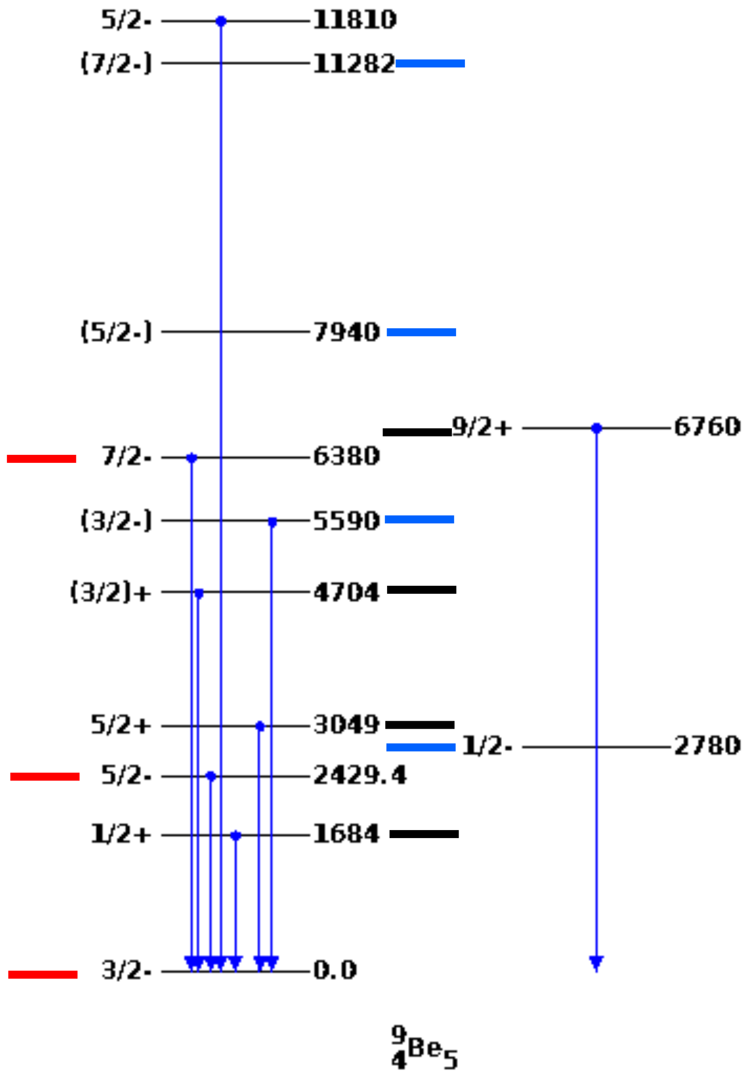
Work in progress: Kyle Godbey, Gaute Hagen, TP preliminary

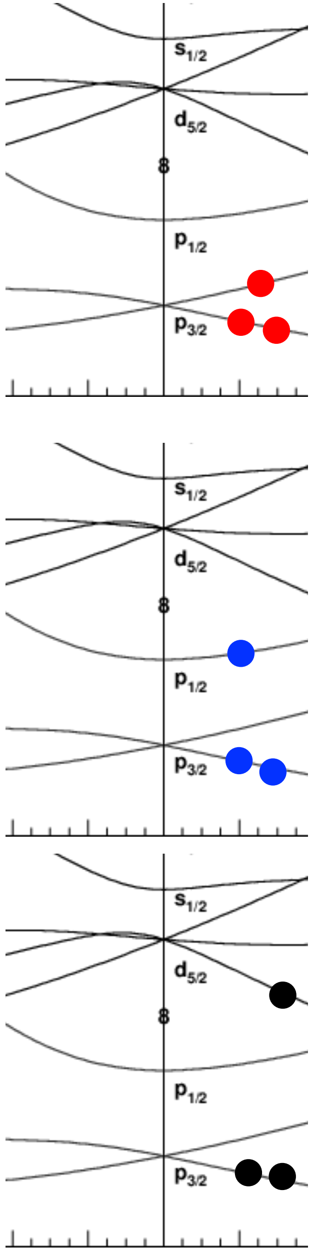




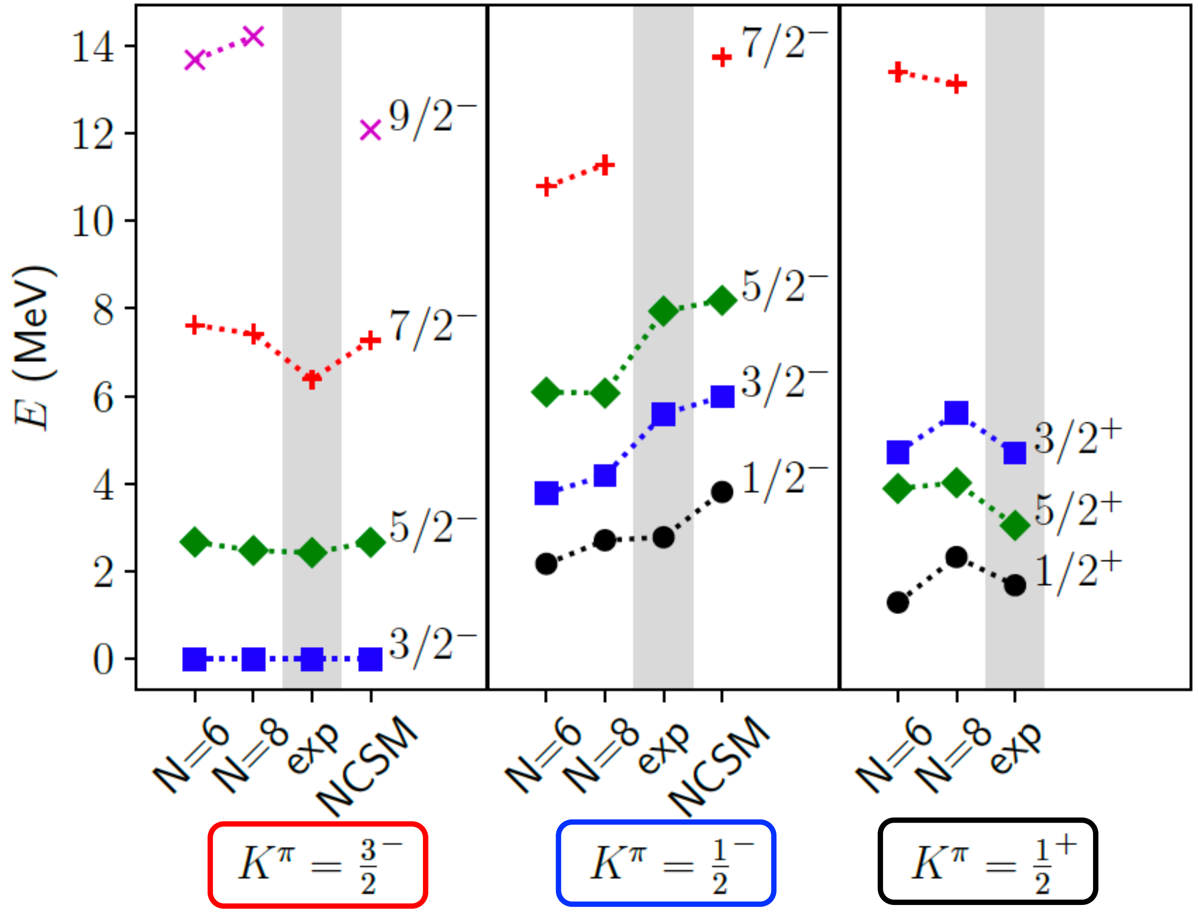
Making sense of spectra in odd-mass nuclei

Looks complicated;
shown data lacks understanding





Zhonghao Sun et al., in preparation
Hartree-Fock computations yield deformed reference
Coupled-cluster + projection yields bands



NCSM from Caprio, Maris, Vary & Smith,
Int. J. Mod. Phys. E 24, 1541002 (2015)

Summary

- The discrepancy between (e,e') and (γ,n) experiments regarding $B(M1)$ in ^{48}Ca is puzzling
- Our ab initio computations based on chiral effective field theory, including treatment of the state as a resonance, yield $7\mu_N^2 < B(M1) < 10\ \mu_N^2$
  - Two-body currents do not yield quenching of $B(M1)$
  - Similar to what was found in light nuclei
- Resolution of this puzzle will impact ab initio computations and/or theory of neutrino-nucleus reactions relevant for supernova signals and dynamics

- Dusted off time-dependent coupled-cluster code; response functions soon; want to join the movie-making business later
- Odd mass deformed nuclei

Thank you!