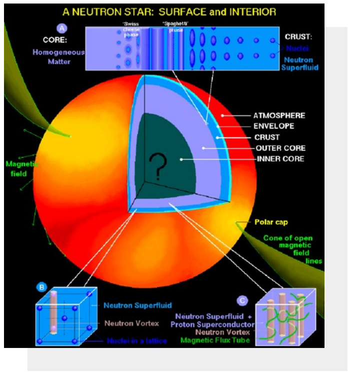
Phenomenology and *ab initio* for heavy and light nuclei

Alex Gezerlis

UNIVERSITY OF GUELPH

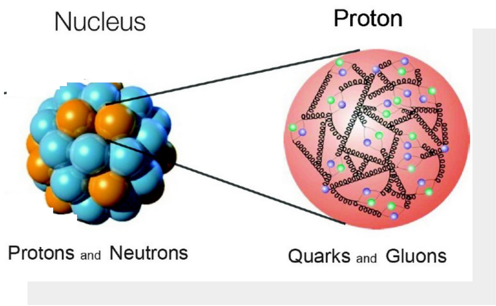
Theory Canada 17
University of Regina
June 7, 2025

Outline

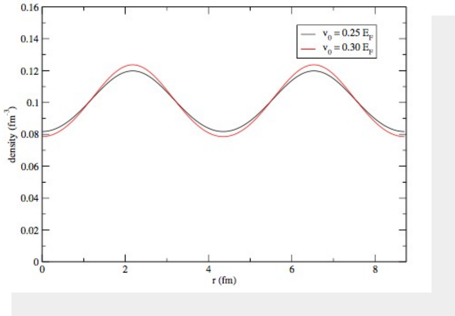


Credit: Dany Page

Motivation

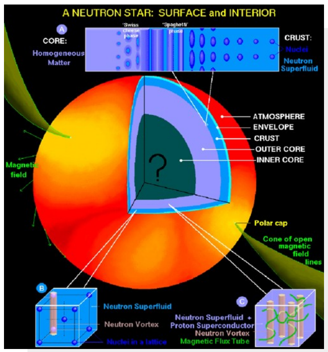


Nuclear methods



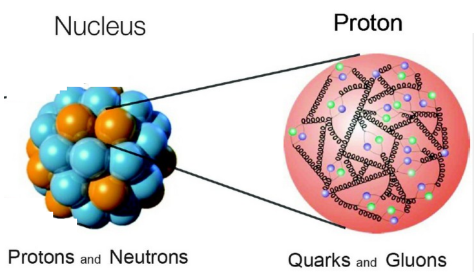
Recent results

Outline

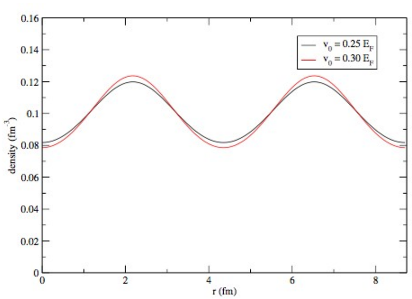


Credit: Dany Page

Motivation



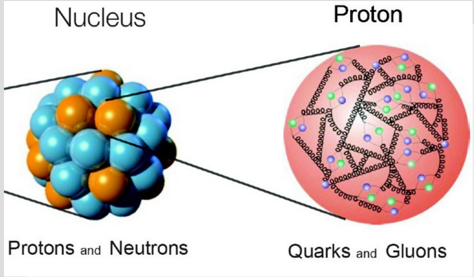
Nuclear methods



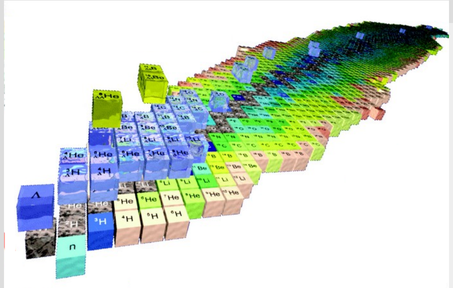
Recent results

Physical systems studied

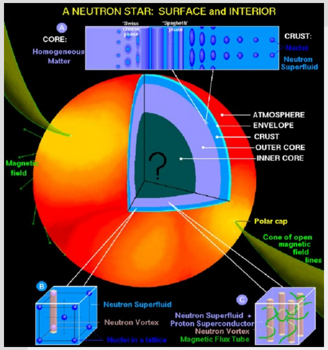
Nuclear forces



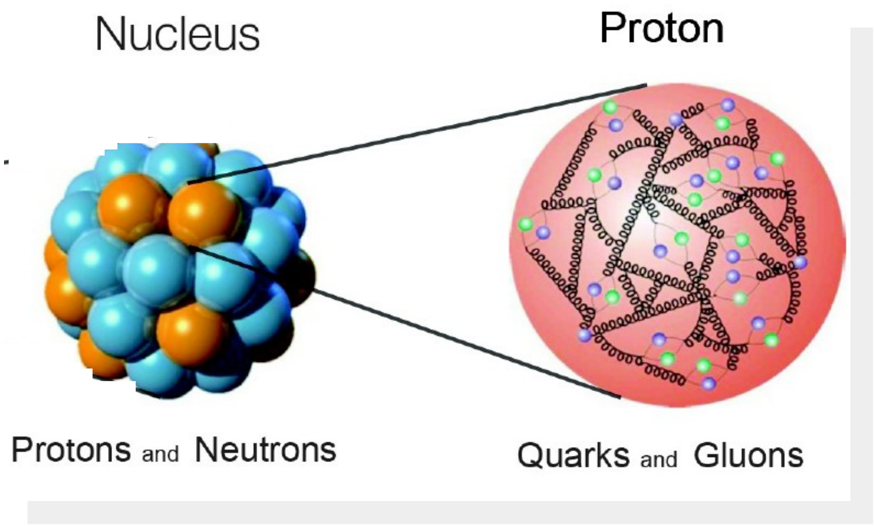
Nuclear structure



Nuclear astrophysics

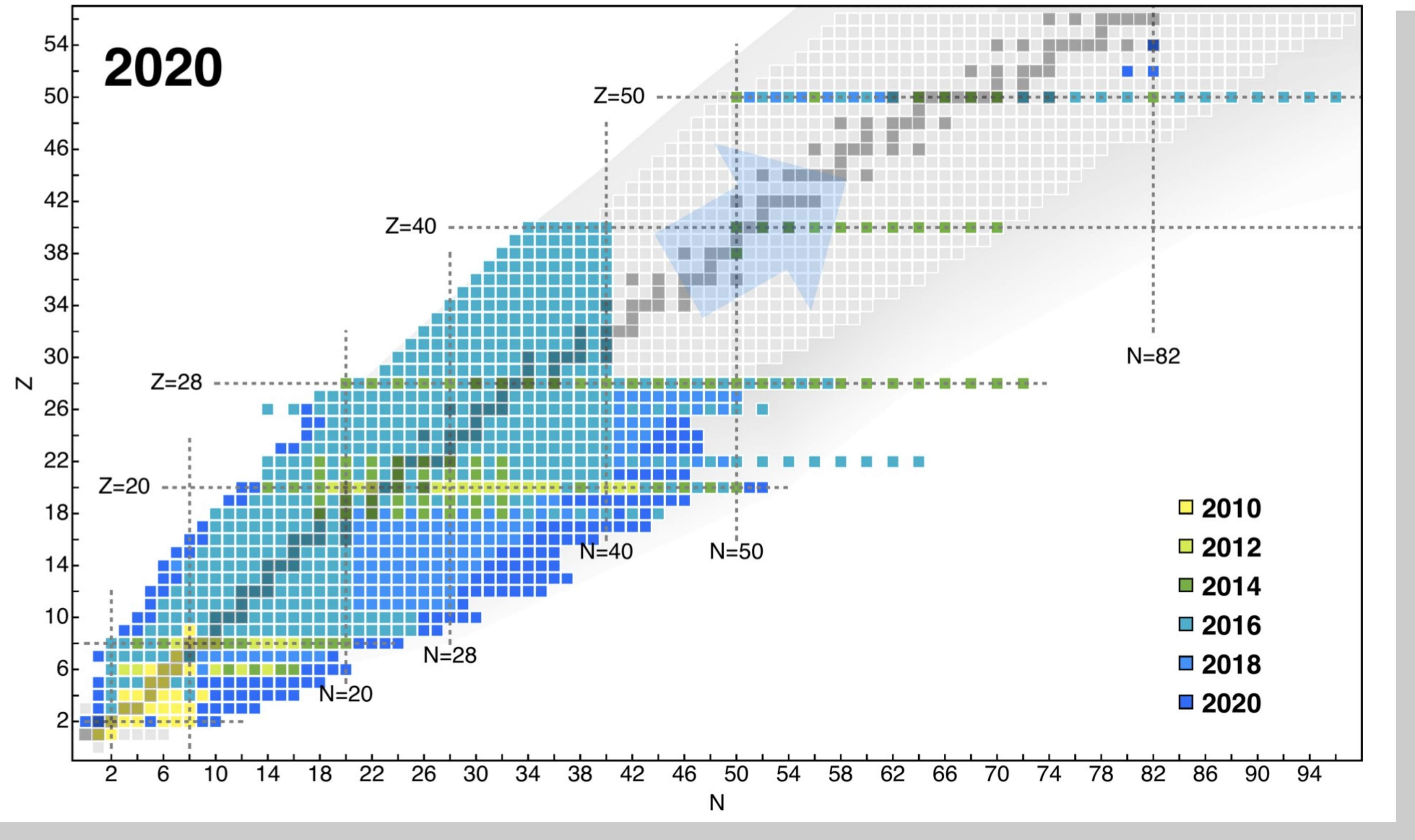


Key system: few nucleons



- No unique nuclear potential
- Preferable to use combination of phenomenological (high-quality) and more modern (conceptually clean) approach
- Desirable to make contact with underlying level
- New era, where practitioners design interactions themselves

Key system: nuclei

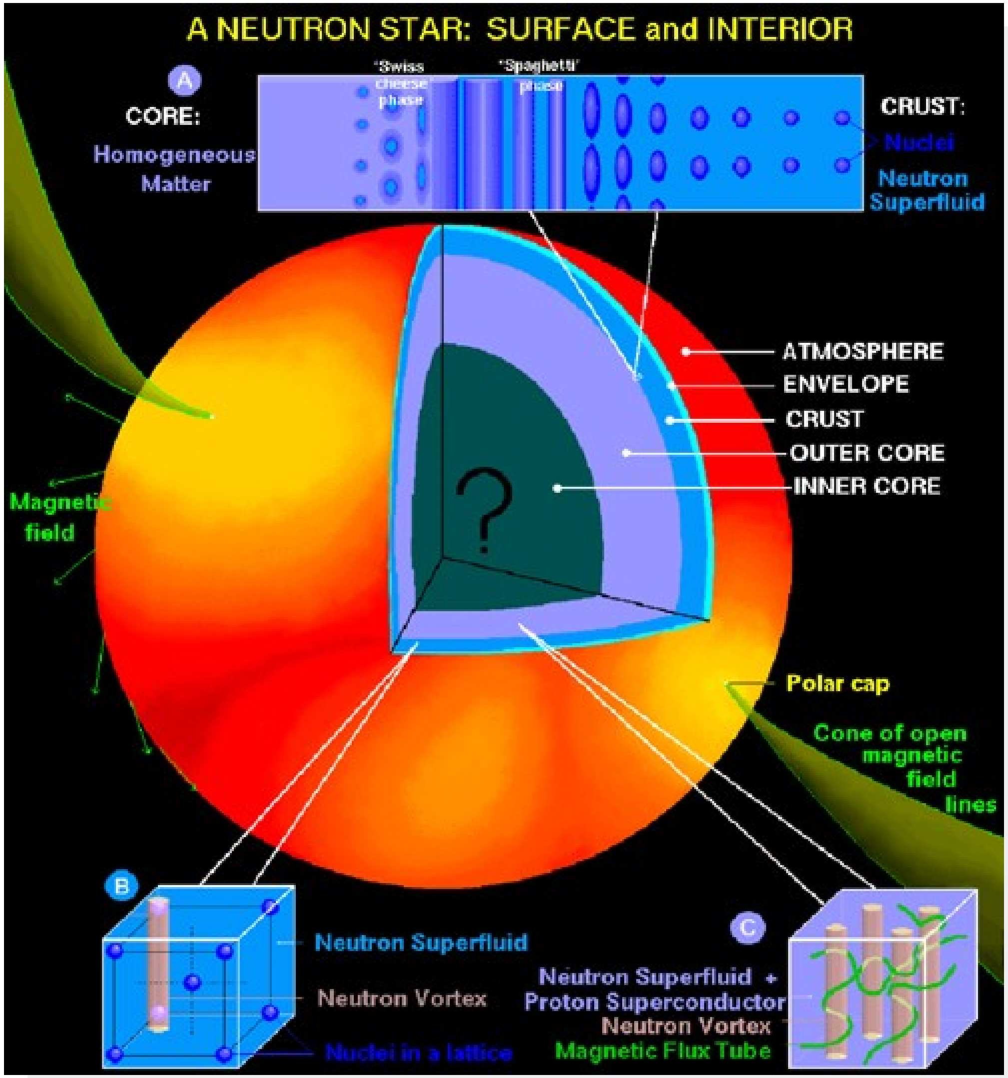


Credit: Heiko Hergert

- Lots of recent progress
- Open-shell nuclei are the current frontier

- Goal is to study nuclei *from first principles* (when possible)

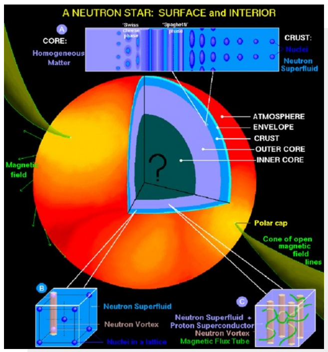
Key system: neutron stars



Credit: Dany Page

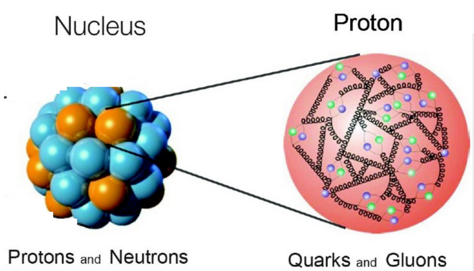
- Ultra-dense: 1.4 solar masses (or more) within a radius of 10 kilometres
- Terrestrial-like (outer layers) down to exotic (core) behaviour
- Observationally probed, i.e., not experimentally accessible
- Goal is to study neutron stars *from first principles* (when possible)

Outline

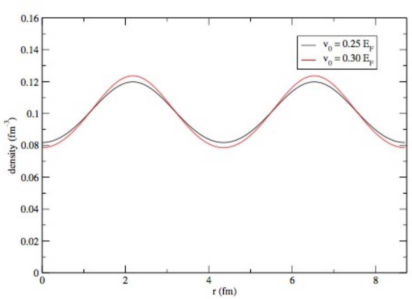


Credit: Dany Page

Motivation

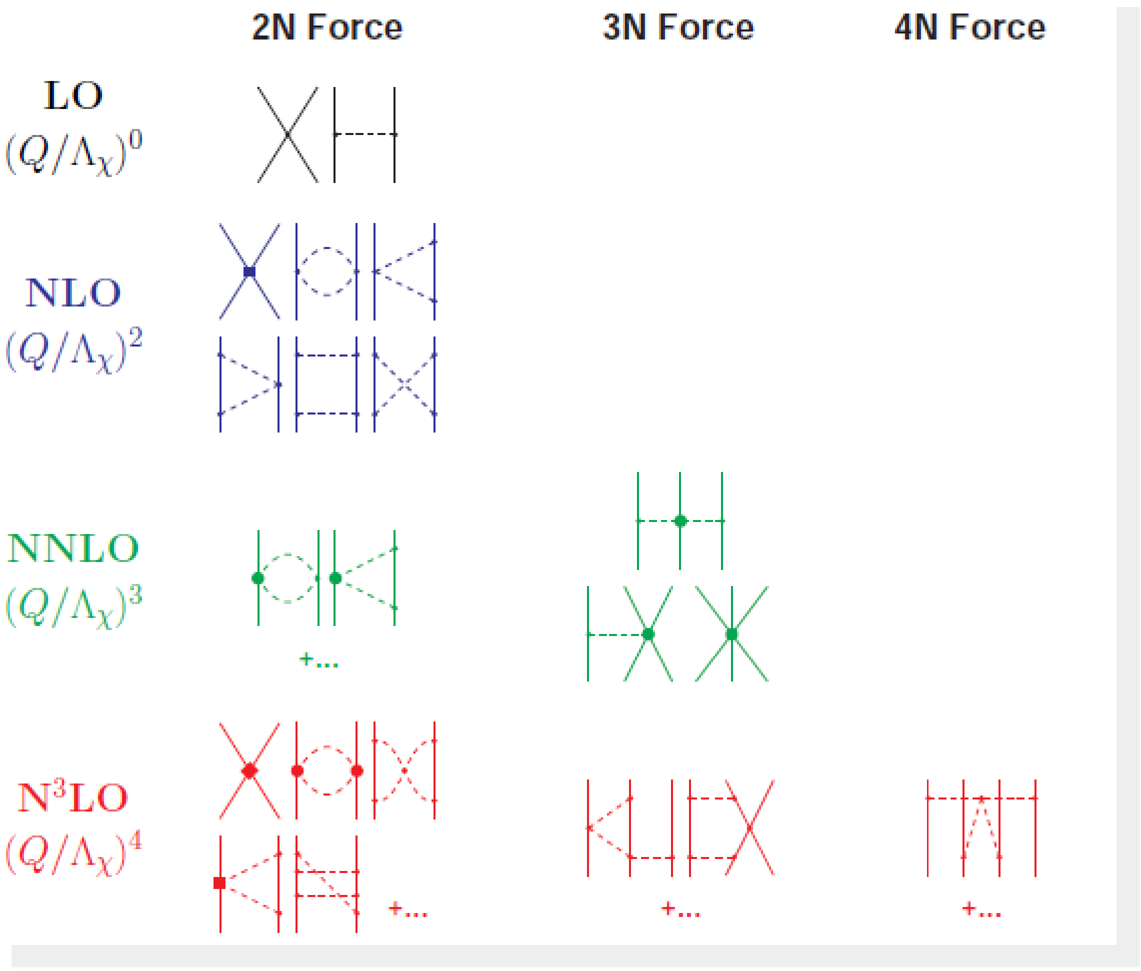


Nuclear methods



Recent results

Nuclear interactions



- Attempts to connect with underlying theory (QCD)
- Low-momentum expansion
- Naturally emerging many-body forces
- Low-energy constants from experiment or lattice QCD
- Now available in non-local, local, or semi-local varieties
- Power counting's relation to renormalization actively investigated

S. Weinberg, U. van Kolck, E. Epelbaum, N. Kaiser ...

But even with the interaction in place, how do you solve the many-body problem?

Nuclear many-body problem

UNIVERSITY OF GUELPH

$$H\Psi = E\Psi$$

where $$H = \sum_i K_i + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk}$$

Wave function depends on coordinates, spin projections, and isospin projections, so we are faced with a large number of complex coupled second-order differential equations

Nuclear many-body methods

- Phenomenological (fit to A-body experiment)
- Ab initio (fit to few-body experiment)

Two complementary approaches

UNIVERSITY OF GUELPH

Phenomenological (fit to A-body experiment)

- *Shell model*
  mainstay of nuclear physics, still very important
- *Hartree-Fock/Hartree-Fock-Bogoliubov (HF/HFB)*
  mean-field theory, a priori inapplicable, unreasonably effective
- *Energy-density functionals (EDF)*
  like mean-field but with wider applicability

Two complementary approaches

UNIVERSITY OF GUELPH

Phenomenological (fit to A-body experiment)

- *Shell model*
  mainstay of nuclear physics, still very important

- *Hartree-Fock/Hartree-Fock-Bogoliubov (HF/HFB)*
  mean-field theory, a priori inapplicable, unreasonably effective

- *Energy-density functionals (EDF)*
  like mean-field but with wider applicability

Two complementary approaches

UNIVERSITY OF GUELPH

Ab initio (fit to few-body experiment)

- *Quantum Monte Carlo (QMC)*
  stochastically solve the many-body problem "exactly"
- *Perturbative Theories (PT)*
  first few orders only
- *Resummation schemes (e.g. SCGF)*
  selected class of diagrams up to infinite order
- *Coupled cluster (CC)*
  generate np-nh excitations of a reference state
- *No-core shell model (NCSM)*
  fully ab initio, in contradistinction to traditional SM

Two complementary approaches

UNIVERSITY OF GUELPH

Ab initio (fit to few-body experiment)

- *Quantum Monte Carlo (QMC)*
  stochastically solve the many-body problem “exactly”

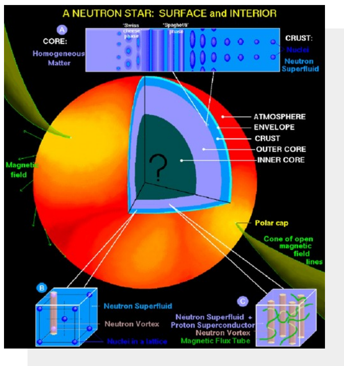
- *Perturbative Theories (PT)*
  first few orders only

- *Resummation schemes (e.g. SCGF)*
  selected class of diagrams up to infinite order

- *Coupled cluster (CC)*
  generate np-nh excitations of a reference state

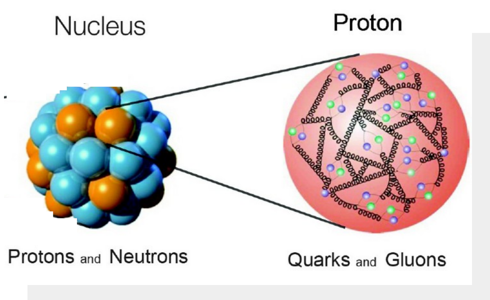
- *No-core shell model (NCSM)*
  fully ab initio, in contradistinction to traditional SM

Outline

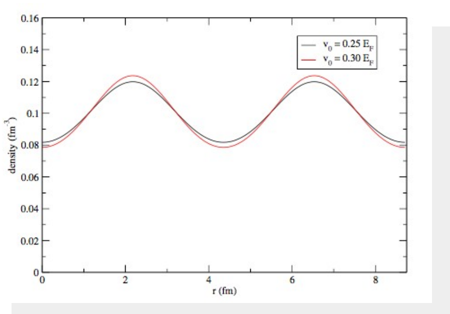


Credit: Dany Page

Motivation



Nuclear methods



Recent results

Recent results

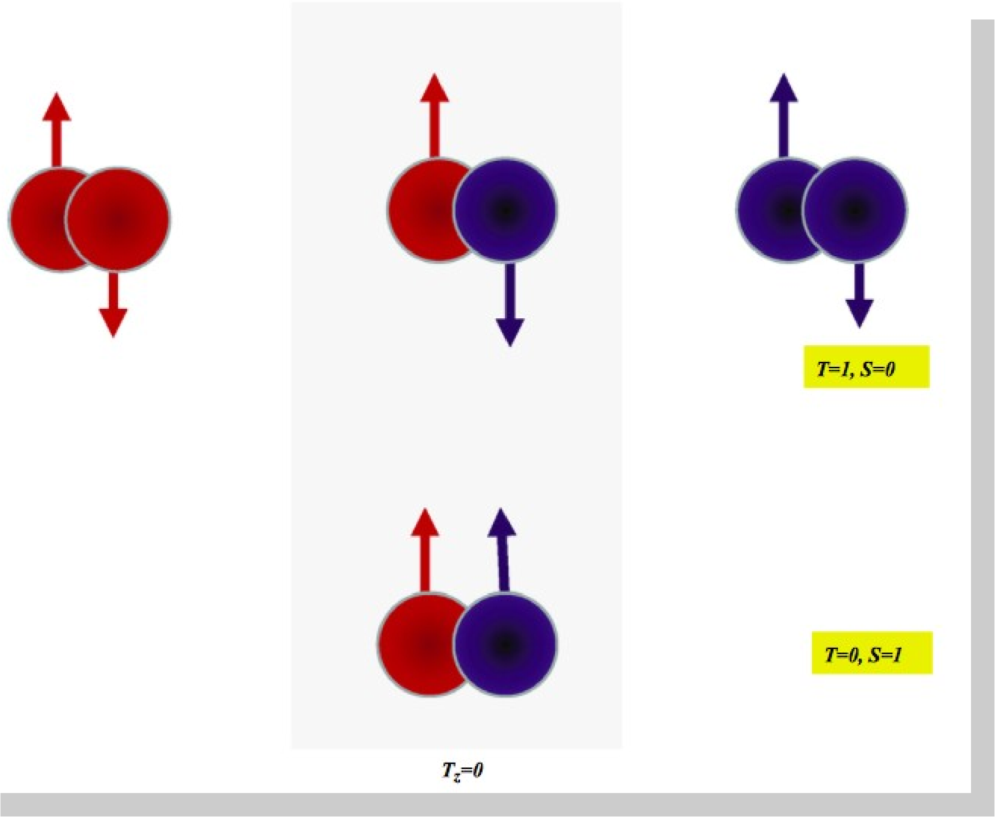
- Mixed-spin pairing in heavy nuclei
- Neural-network wave functions for light nuclei

Mixed-spin pairing in heavy nuclei

G. Palkanoglou, M. Stuck, and A. Gezerlis, Phys. Rev. Lett. **134**, 032501 (2025)

G. Palkanoglou and A. Gezerlis, arXiv:2505.08879

Types of pairs in nuclei



S. Frauendorf and A. O. Macchiavelli, Prog. Nucl. Part. Phys. **78**, 24 (2014)

Deuteron-like pairing

central "paradox"

- *np* interaction stronger than *nn* and *pp* interaction (*there is no bound dineutron in vacuum*)
- However, known nuclei exhibit *nn* and *pp* pairing.

Deuteron-like pairing

UNIVERSITY OF GUELPH

central "paradox"

- *np* interaction stronger than *nn* and *pp* interaction (*there is no bound dineutron in vacuum*)
- However, known nuclei exhibit *nn* and *pp* pairing.

Possible answer I:

- Isospin polarization discourages spin-triplet pairing: look at N=Z nuclei

A. L. Goodman, Phys. Rev. C **58**, R3051 (1998)

A. O. Macchiavelli *et al.*, Phys. Rev. C **61**, 041303(R) (2000)

R. Chasman, Phys. Lett. B **524**, 81 (2002)

Possible answer II:

- Spin-orbit field interferes with spin-triplet pairing more: look at heavy nuclei

A. Poves and G. Martinez-Pinedo, Phys. Lett. B **430**, 203 (1998)

G. F. Bertsch and Y. L. Luo, Phys. Rev. C **81**, 064320 (2010)

S. Baroni, A. O. Macchiavelli, A. Schwenk, Phys. Rev. C 8**1**, 064308 (2010)

Hamiltonian

UNIVERSITY OF GUELPH

$$\hat{H} = \sum_i \langle i|H_{sp}|j\rangle a_i^\dagger a_j + \sum_{i>j,k>l} \langle ij|v|kl\rangle a_i^\dagger a_j^\dagger a_l a_k$$

- H_{sp} : kinetic + potential well + spin-orbit
- $\langle ij|v|kl\rangle$ contact pairing interaction in 6 channels

$$\langle ij|v|kl\rangle = \frac{1}{4}\langle ij|(3v_t + v_s + (v_t - v_s)\vec{\sigma}\cdot\vec{\sigma}')\delta^{(3)}(\vec{r} - \vec{r}')P_{L=0}|kl\rangle$$

where v_s and v_t are fit (and varied)

Hartree-Fock-Bogoliubov theory

- Applying the Bogoliubov U and V we go to the quasiparticle representation

- The ordinary and anomalous densities are:

  $\rho = V^* V^T$ and $\kappa = V^* U^T$

- Hartree-Fock-Bogoliubov equations:

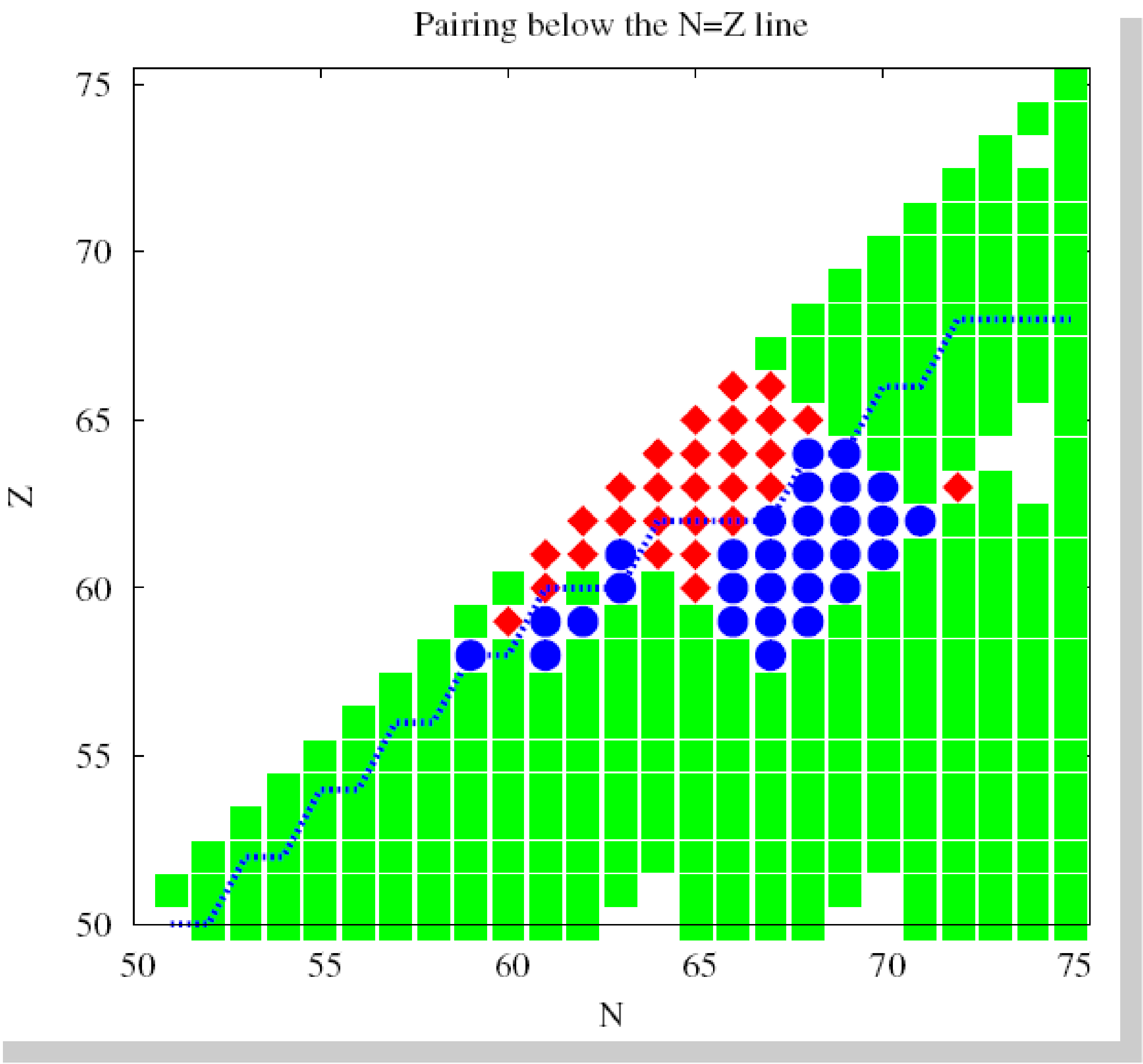
$$\begin{bmatrix} h' & \Delta \\ -\Delta^* & -h'^* \end{bmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = \begin{pmatrix} U_k \\ V_k \end{pmatrix} E_k$$

where $h = \varepsilon + \Gamma$ and the interaction is buried inside

$$\Gamma_{ij} = \sum_{kl} \bar{v}_{iljk} \rho_{kl}$$

$$\Delta_{ij} = \frac{1}{2} \sum_{kl} \bar{v}_{ijkl} \kappa_{kl}$$

Pairing in heavy nuclei



Correlation energies

- Blue line: proton drip
- Green: spin-singlet
- Red: spin-triplet
- Blue: mixed-spin
- Spin-triplet pairing persists off N=Z line
- Mixed-spin pairing appears to be energetically stable (note: no deformation)

A. Gezerlis, G. F. Bertsch, and Y. L. Luo, Phys. Rev. Lett. **106**, 252502 (2011)

What about deformation?

To go beyond, take a deformed Woods-Saxon well:

$$\psi_{nl_z}(\rho,\phi,z) = \frac{e^{l_z\phi}}{\sqrt{2\pi}}\frac{u(\rho,z)}{\sqrt{\rho}}$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial\rho}^2 + \frac{\partial}{\partial z}^2\right)u + \left[V_{\mathrm{WS}}(\rho,z) + \frac{\hbar^2}{2m}\frac{l_z}{\rho^2} - \frac{\hbar^2}{2m}\frac{1}{4\rho^2}\right]u = E_{nl_z}u$$

What about deformation?

UNIVERSITY OF GUELPH

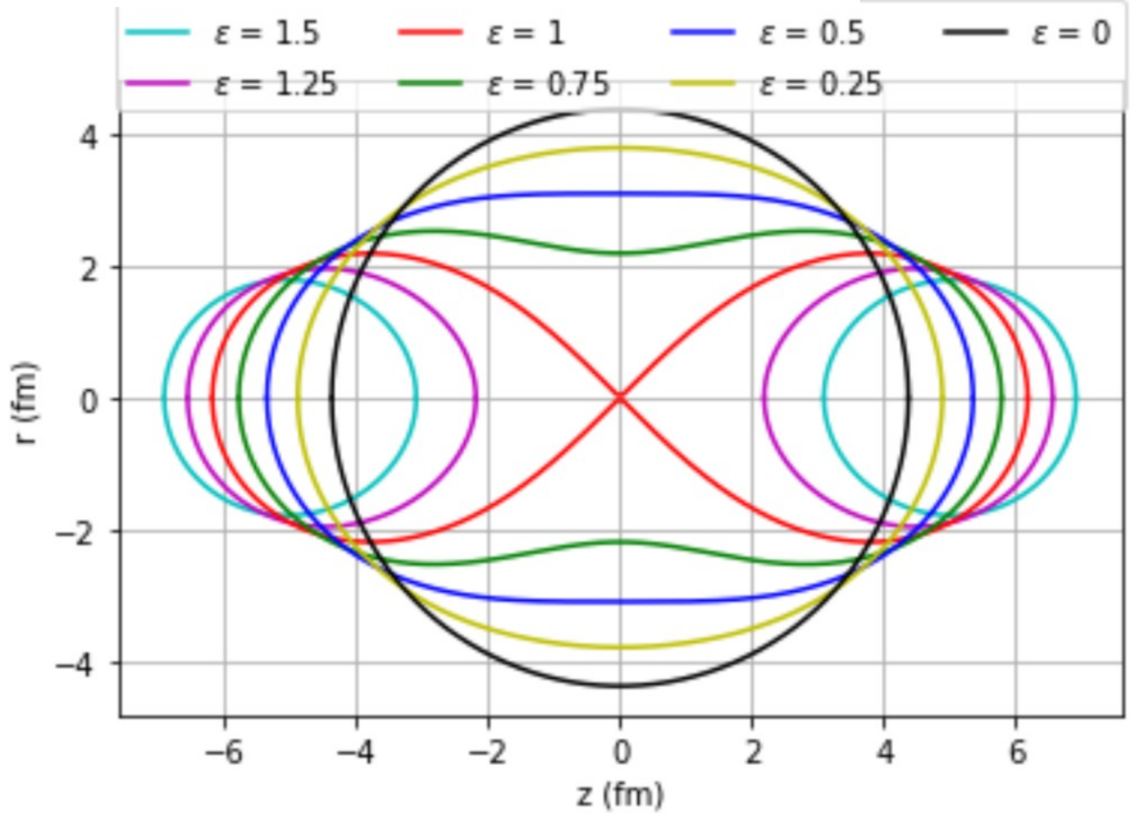
To go beyond, take a deformed Woods-Saxon well:

$$\psi_{nl_z}(\rho,\phi,z) = \frac{e^{l_z\phi}}{\sqrt{2\pi}}\frac{u(\rho,z)}{\sqrt{\rho}}$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial\rho}^2 + \frac{\partial}{\partial z}^2\right)u + \left[V_{\mathrm{WS}}(\rho,z) + \frac{\hbar^2}{2m}\frac{l_z}{\rho^2} - \frac{\hbar^2}{2m}\frac{1}{4\rho^2}\right]u = E_{nl_z}u$$

$$V_{\mathrm{WS}}(\rho,z) = \frac{V_0}{1+e^{d(\rho,z)/a}}$$

Surface is a Cassini oval:



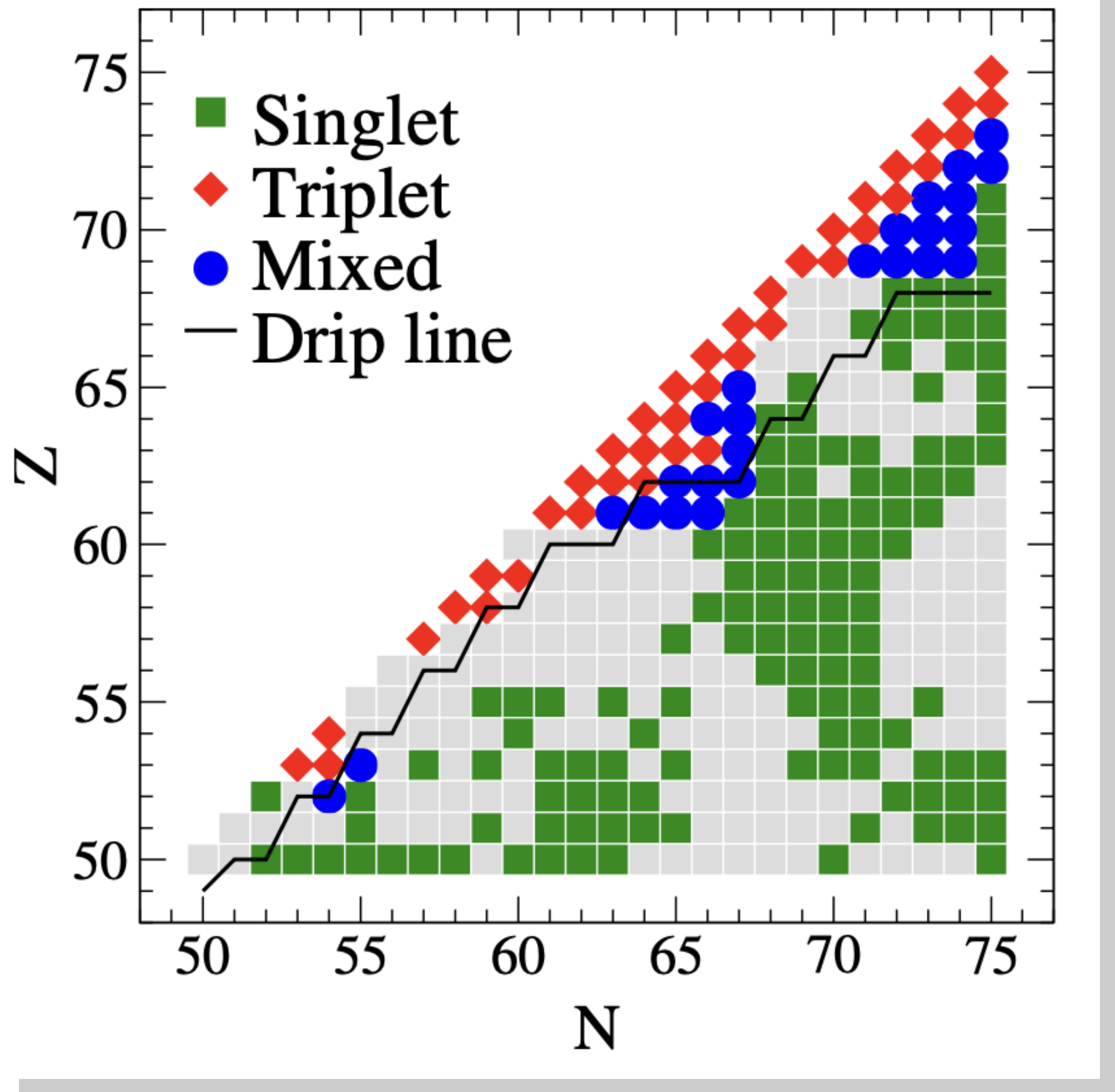
Deformation and exotic pairing

UNIVERSITY OF GUELPH

Deformation impacts but does not kill mixed-spin pairing:

- Quadrupole deformation is main factor

- For N=Z deformation actually *enhances* spin-triplet pairing



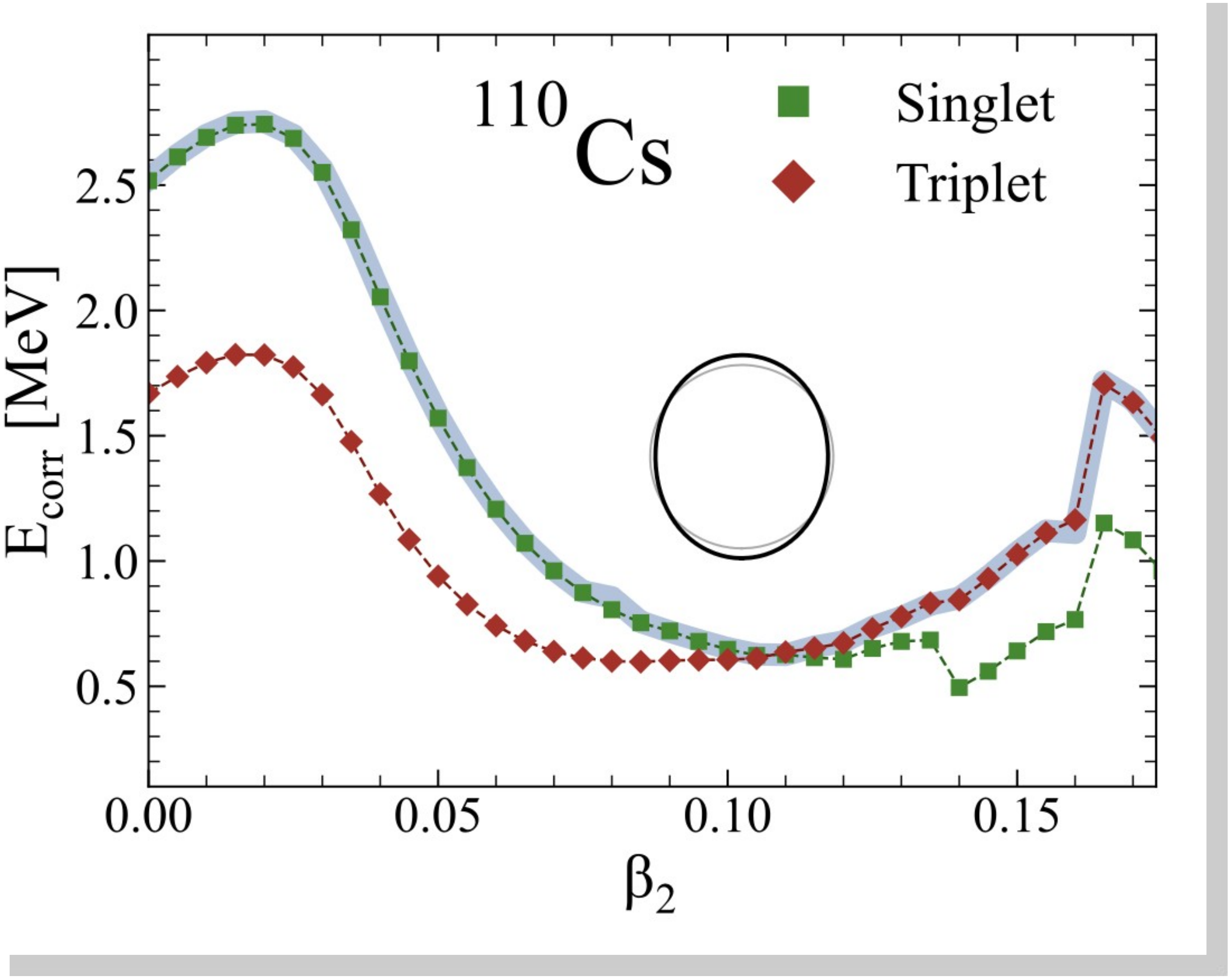
G. Palkanoglou, M. Stuck, and A. Gezerlis, Phys. Rev. Lett. **134**, 032501 (2025)

Deformation and exotic pairing

Vary quadrupole deformation and compare constrained with unconstrained runs.

Deformation impacts the surface and therefore the effect of spin-orbit.

But spin-triplet pairs move to the interior of the nucleus and are unimpacted.



G. Palkanoglou and A. Gezerlis, arXiv:2505.08879

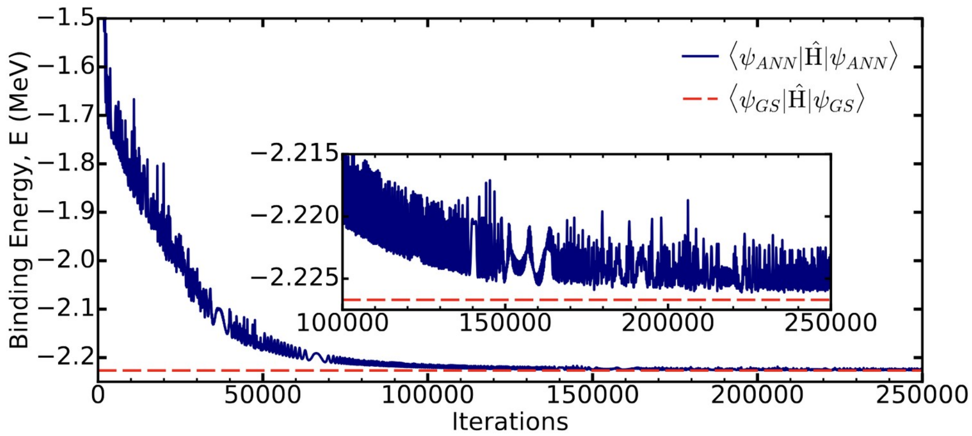
Neural-network wave functions for light nuclei

P. Weng, A. Gezerlis, and J. Holt, arXiv:2505.11442

Earlier work

UNIVERSITY OF GUELPH

Deuteron



J. W. T. Keeble and A. Rios,
Phys. Lett. B **809**, 135743 (2020)

Light nuclei

	Λ	VMC-ANN	VMC-JS	GFMC	GFMC_c
^{2}H	4 fm^{-1}	−2.224(1)	−2.223(1)	−2.224(1)	-
	6 fm^{-1}	−2.224(4)	−2.220(1)	−2.225(1)	-
^{3}H	4 fm^{-1}	−8.26(1)	−7.80(1)	−8.38(2)	−7.82(1)
	6 fm^{-1}	−8.27(1)	−7.74(1)	−8.38(2)	−7.81(1)
^{4}He	4 fm^{-1}	−23.30(2)	−22.54(1)	−23.62(3)	−22.77(2)
	6 fm^{-1}	−24.47(3)	−23.44(2)	−25.06(3)	−24.10(2)

C. Adams, G. Carleo, A. Lovato, N. Rocco,
Phys. Rev. Lett. **127**, 022502 (2021)

N.B. Limited to pionless Hamiltonian

Neural networks for light nuclei

UNIVERSITY OF GUELPH

Spin-isospin correlations

$$|\psi\rangle = \mathcal{S}\prod_{i<j}\left(1+\sum_{\mathrm{x}} u_{ij}^{(\mathrm{x})}\hat{O}_{ij}^{(\mathrm{x})}\right) f_{ij}^{(c)}|\Phi\rangle$$

$$|\psi\rangle \to \left(1+\sum_{i<j<k}\sum_{\mathrm{cyc}}\sum_{\mathrm{x}} \epsilon^{(\mathrm{x})}\hat{V}_{ijk}^{(\mathrm{x})}\right)|\psi\rangle$$

for N2LO chiral Hamiltonian

P. Weng, A. Gezerlis, and J. Holt, arXiv:2505.11442

Neural networks for light nuclei

UNIVERSITY OF GUELPH

Nearly reproduces GFMC results
already at the VMC level

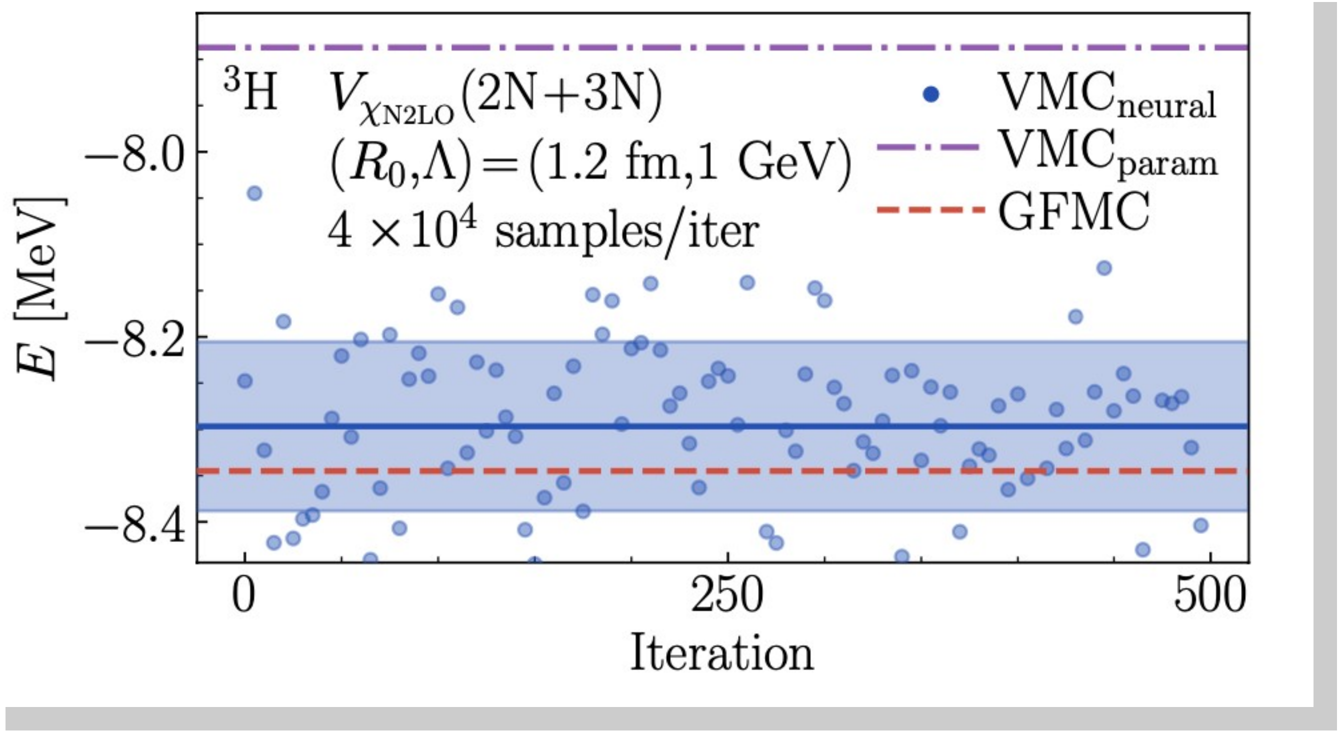
$E = E_k + V_{\chi N^2LO}(2N)$				
	R_0 [fm]	E_{neural} [MeV]	E_{GFMC} [MeV]	$\|\Delta E\|/\|E_{GFMC}\|$
^3H	1.0	-7.338 ± 0.008	-7.554 ± 0.007	2.9%
	1.1	-7.500 ± 0.006	-7.625 ± 0.005	1.6%
	1.2	-7.678 ± 0.005	-7.740 ± 0.005	0.8%
^2H	1.0	-2.217 ± 0.005	-2.21 ± 0.02	0.3%
	1.2	-2.212 ± 0.004	-2.20 ± 0.03	0.5%

P. Weng, A. Gezerlis, and J. Holt, arXiv:2505.11442

Neural networks for light nuclei

UNIVERSITY OF GUELPH

Dramatic improvement over standard/parametric VMC employed before, e.g., AFDMC



P. Weng, A. Gezerlis, and J. Holt, arXiv:2505.11442

Conclusions

UNIVERSITY OF GUELPH

- Rich connections between physics of nuclei, cold atoms, and compact stars
- Exciting time in terms of interplay between nuclear interactions and many-body approaches
- Ab initio and phenomenology are mutually beneficial
- Mixed-spin pairing is present even after you introduce deformation

Acknowledgments

UNIVERSITY OF GUELPH

Collaborators

Guelph

- Michael Stuck

Texas A&M

- Jeremy Holt
- Pengsheng Weng

TRIUMF

- Georgios Palkanoglou

Acknowledgments

UNIVERSITY OF GUELPH

Funding

NSERC CRSNG

INNOVATION.CA
CANADA FOUNDATION FOR INNOVATION | FONDATION CANADIENNE POUR L'INNOVATION

Ontario
MINISTRY OF RESEARCH AND INNOVATION
MINISTÈRE DE LA RECHERCHE ET DE L'INNOVATION

Collaborators

Guelph

- Michael Stuck

Texas A&M

- Jeremy Holt
- Pengsheng Weng

TRIUMF

- Georgios Palkanoglou