

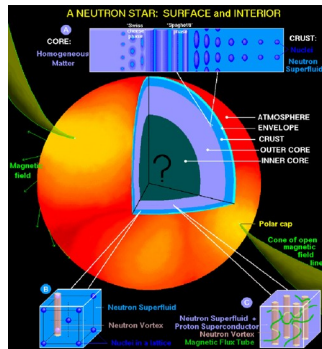
Coexistence of spin-triplet and spin-singlet pairing in heavy nuclei

Alex Gezerlis



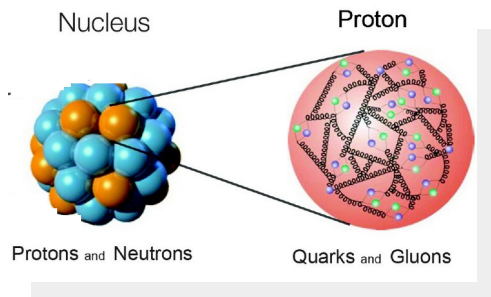
“Ab initio nuclear pairing” workshop
CEA Saclay
May 20, 2025

Outline

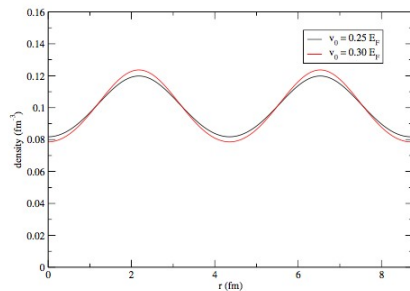


Credit: Dany Page

Motivation



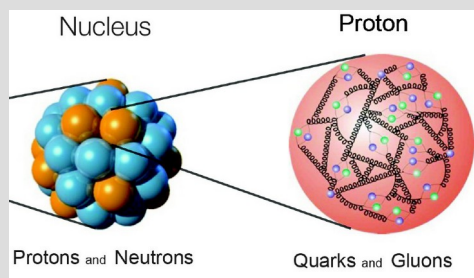
Nuclear methods



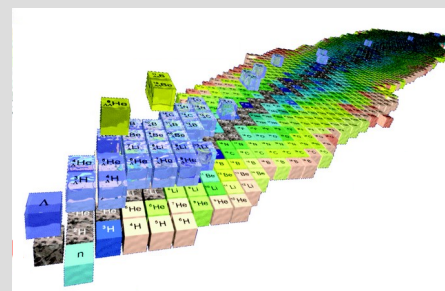
Recent results

Physical systems studied

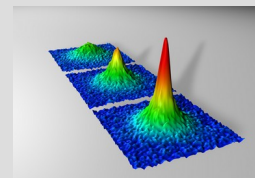
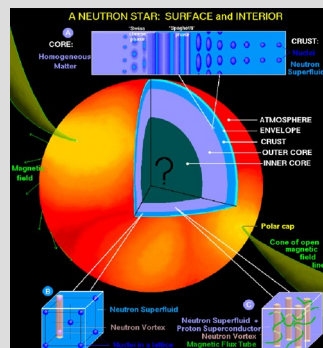
Nuclear forces



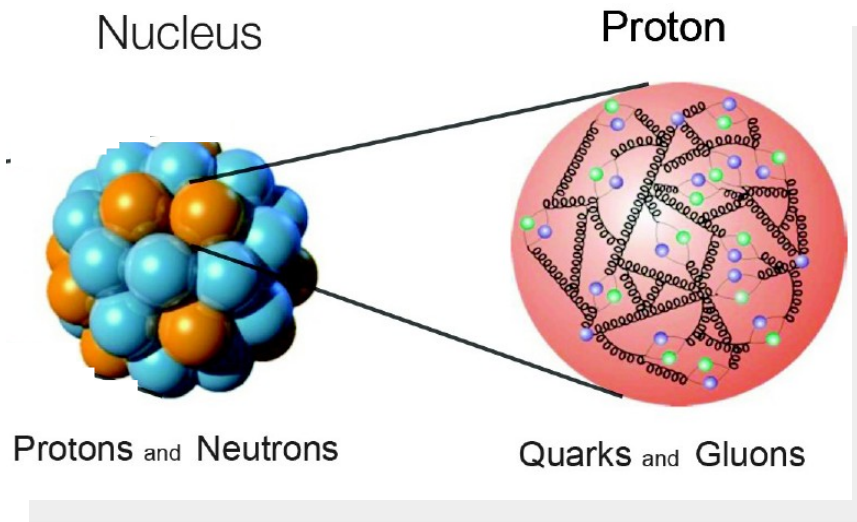
Nuclear structure



Nuclear astrophysics

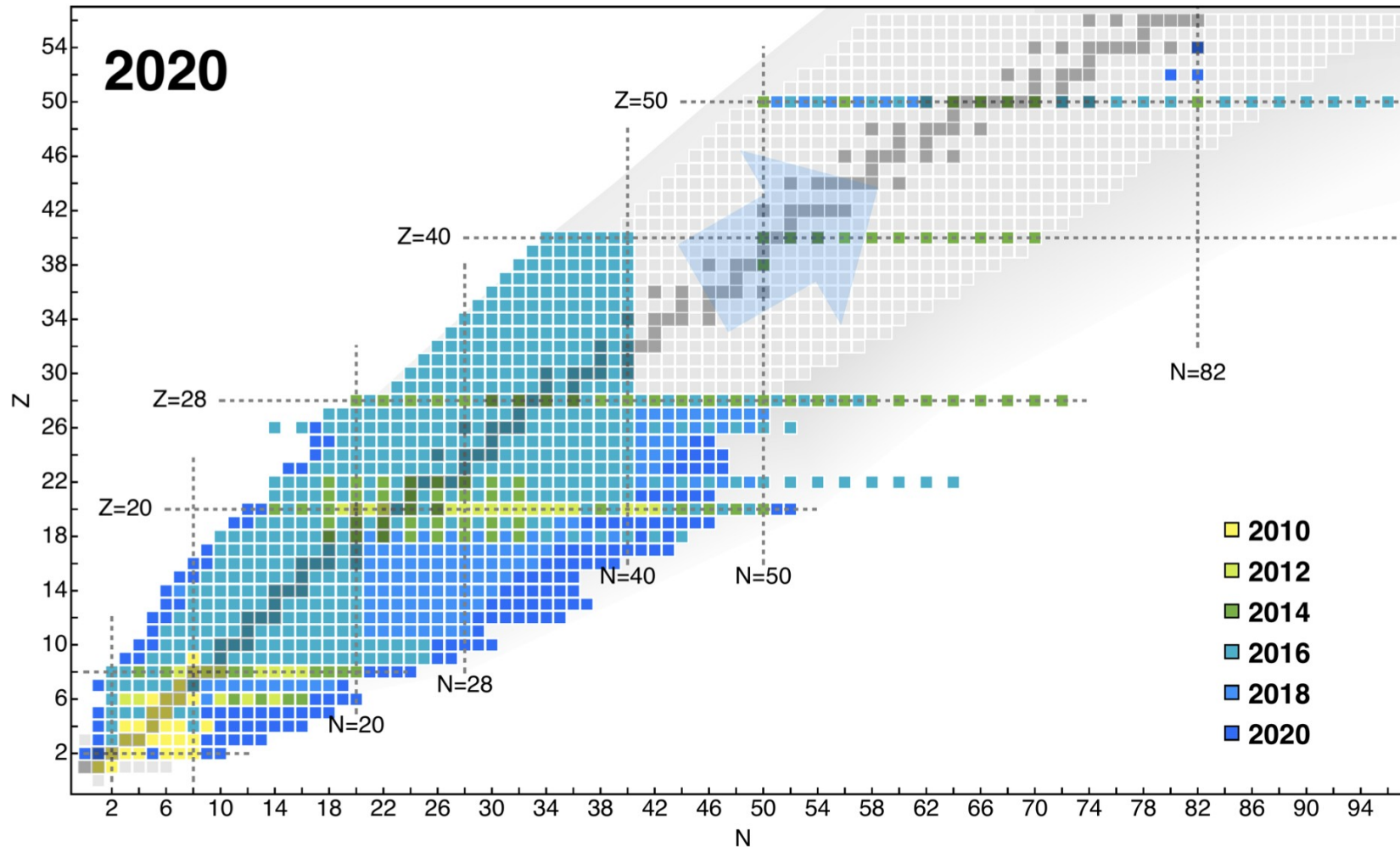


Key system: few nucleons



- 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

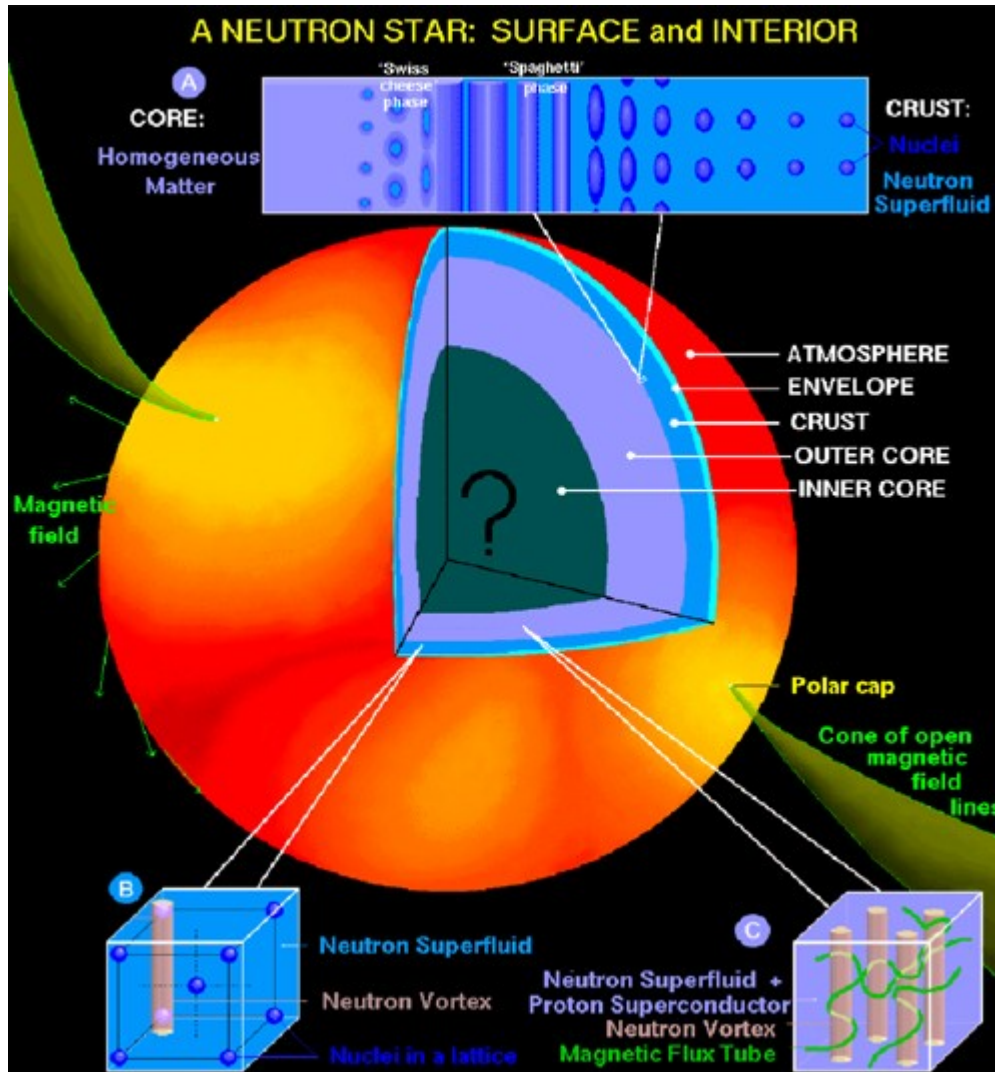
Key system: nuclei



Credit: Heiko Hergert

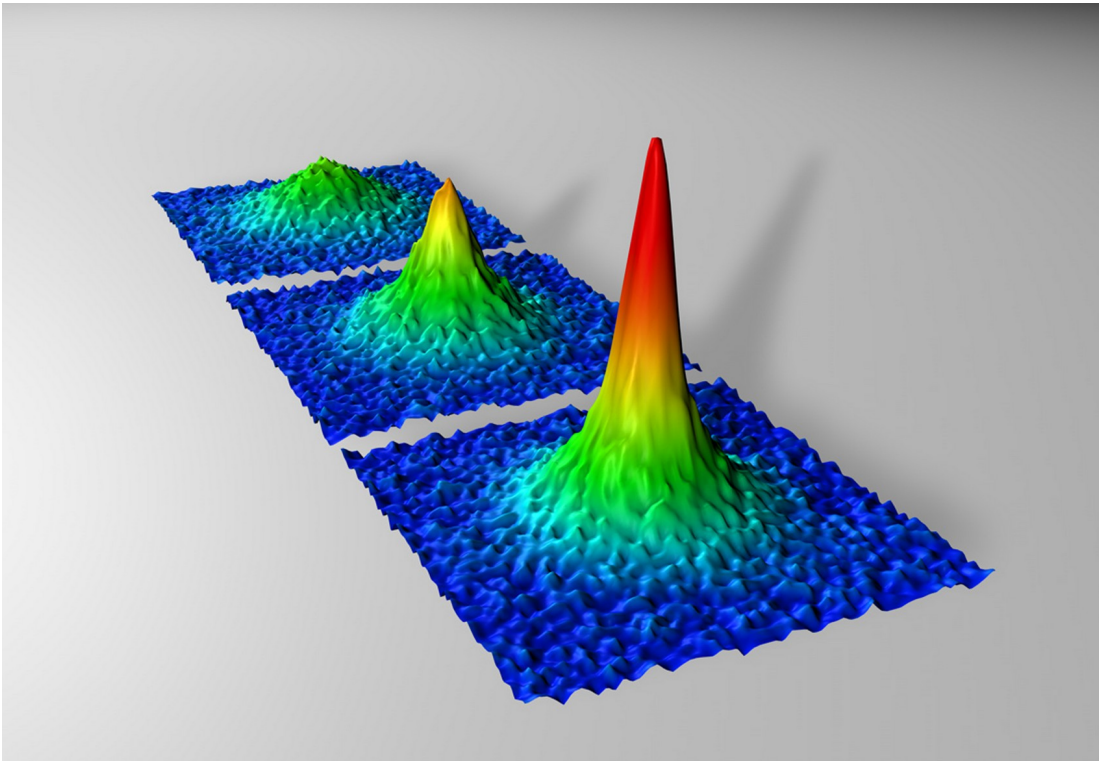
- Lots of recent progress
- Open-shell nuclei are the current frontier
- Goal is to study nuclei *from first principles* (when possible)

Key system: neutron stars



- 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)

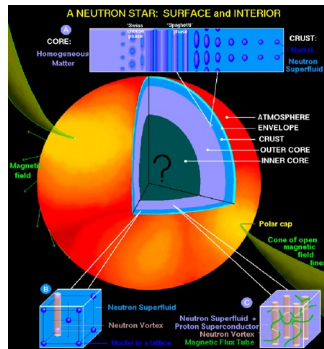
Key system: cold atoms



Credit: University of Colorado

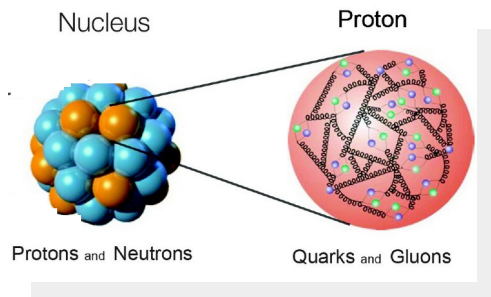
- Starting in the 1990s, it became possible to experimentally probe degenerate bosonic atoms (beyond ^4He)
- Starting in the 2000s, the same happened for fermionic atoms (beyond ^3He)
- These are very cold and strongly interacting (as well as strongly correlated)
- Can be used to simulate other systems, investigating pairing, polarization, polaron physics, many species, reduced dimensionality

Outline

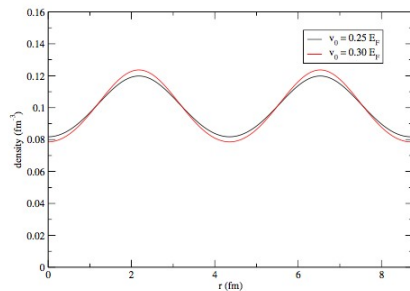


Credit: Dany Page

Motivation

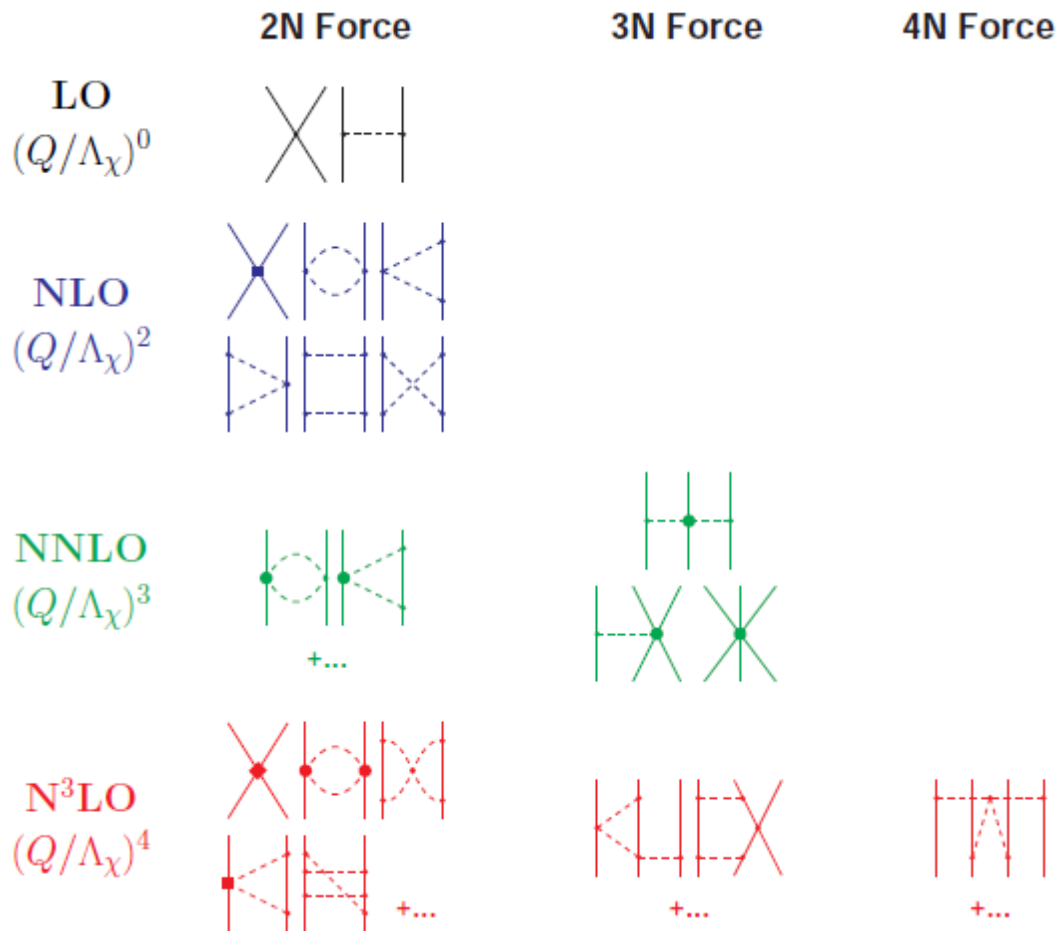


Nuclear methods



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

$$H\Psi = E\Psi$$

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

Phenomenological (fit to A-body experiment)

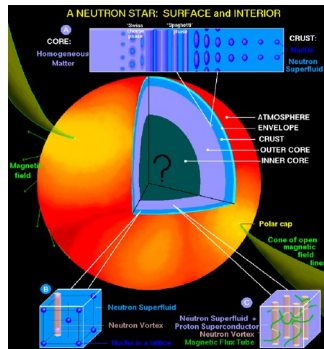
- *Shell model*
mainstay of nuclear physics, still very important
- *Hartree-Fock/Hartree-Fock-Bogoliubov (HF/HFB)*
mean-field theory, a priori inapplicable, unreasonably effective
- *Energy-density functionals (EDF)*
like mean-field but with wider applicability

Two complementary approaches

Ab initio (fit to few-body experiment)

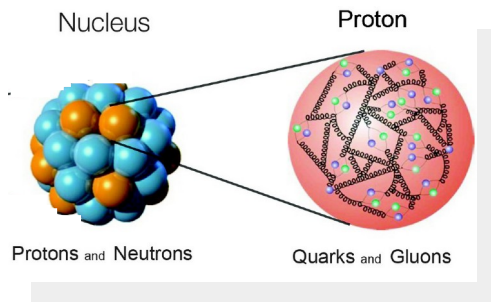
- *Quantum Monte Carlo (QMC)*
stochastically solve the many-body problem “exactly”
- *Perturbative Theories (PT)*
first few orders only
- *Resummation schemes (e.g. SCGF)*
selected class of diagrams up to infinite order
- *Coupled cluster (CC)*
generate np-nh excitations of a reference state
- *No-core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

Outline

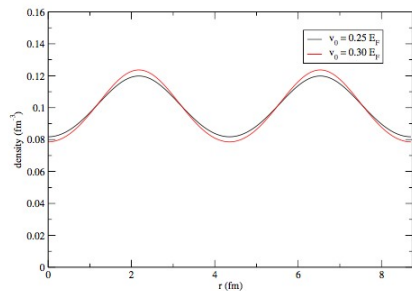


Credit: Dany Page

Motivation



Nuclear methods



Recent results

Recent results

- **Cold atoms with mass imbalance**
- **Mixed-spin pairing in heavy nuclei**
- **Neural-network wave functions for light nuclei**

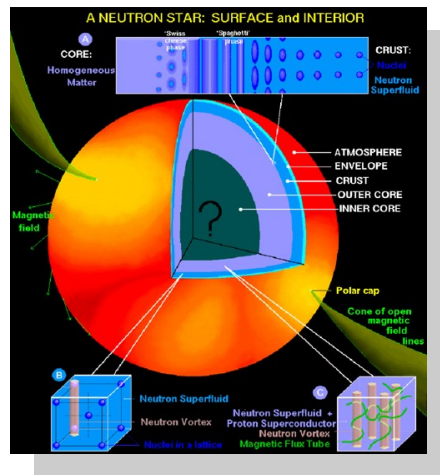
Cold atoms with mass imbalance

S. Gandolfi, R. Curry, and A. Gezerlis, Phys. Rev. A **110**, 043320 (2024)

Connections

Neutron matter

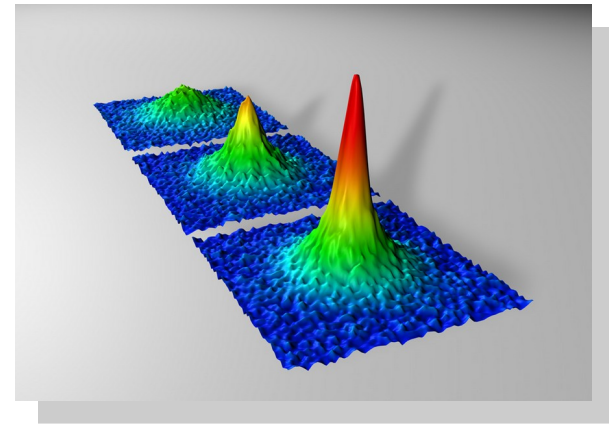
- MeV scale
- $O(10^{57})$ neutrons



Credit: Dany Page

Cold atoms

- peV scale
- $O(10)$ or $O(10^5)$ atoms

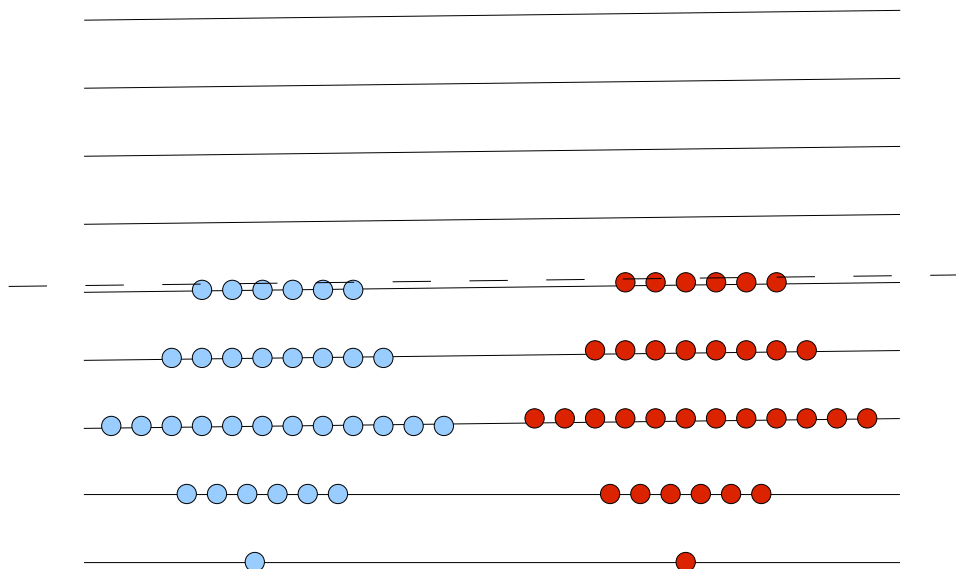


Credit: University of Colorado

For (much) more, see:

G. C. Strinati, P. Pieri, G. Roepke, P. Schuck, and M. Urban,
Physics Reports **738**, 1 (2018).

Fermions



For a single component
(e.g., neutrons with spin-up)
we have a single Slater determinant.

For two components, we separately
place each new particle
in the lowest-available state,
up to the Fermi surface.
(pairing modifies this picture).

If the interaction is zero-range
(contact), there is no s -wave term
(Pauli exclusion principle), but
 p -wave can be present

Mass imbalance

When the two components belong to different atomic species (6Li and 40K experimentally), we also have to consider the mass imbalance:

$$H = \frac{-\hbar^2}{2m_l} \sum_{i=1}^{N_l} \nabla_i^2 + \frac{-\hbar^2}{2m_h} \sum_{j'=1}^{N_h} \nabla_{j'}^2 + \sum_{i < j'} v(r_{ij'})$$

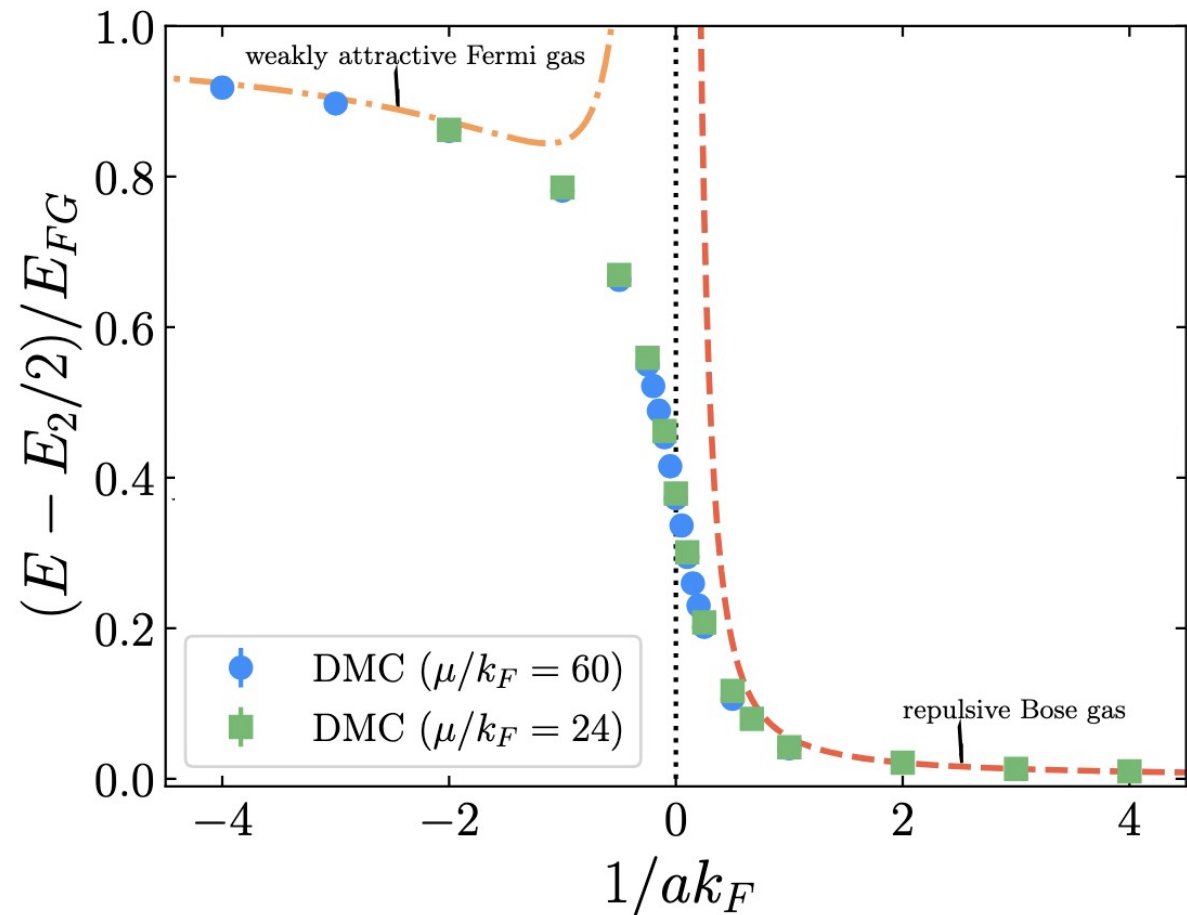
Use diffusion Monte Carlo to capture both strong and weak pairing:

$$\Phi_{\text{BCS}} = \mathcal{A}[\phi(r_{11'})\phi(r_{22'})\dots\phi(r_{N_l N_h})]$$

Mass imbalance

6Li and 40K
BCS-BEC crossover

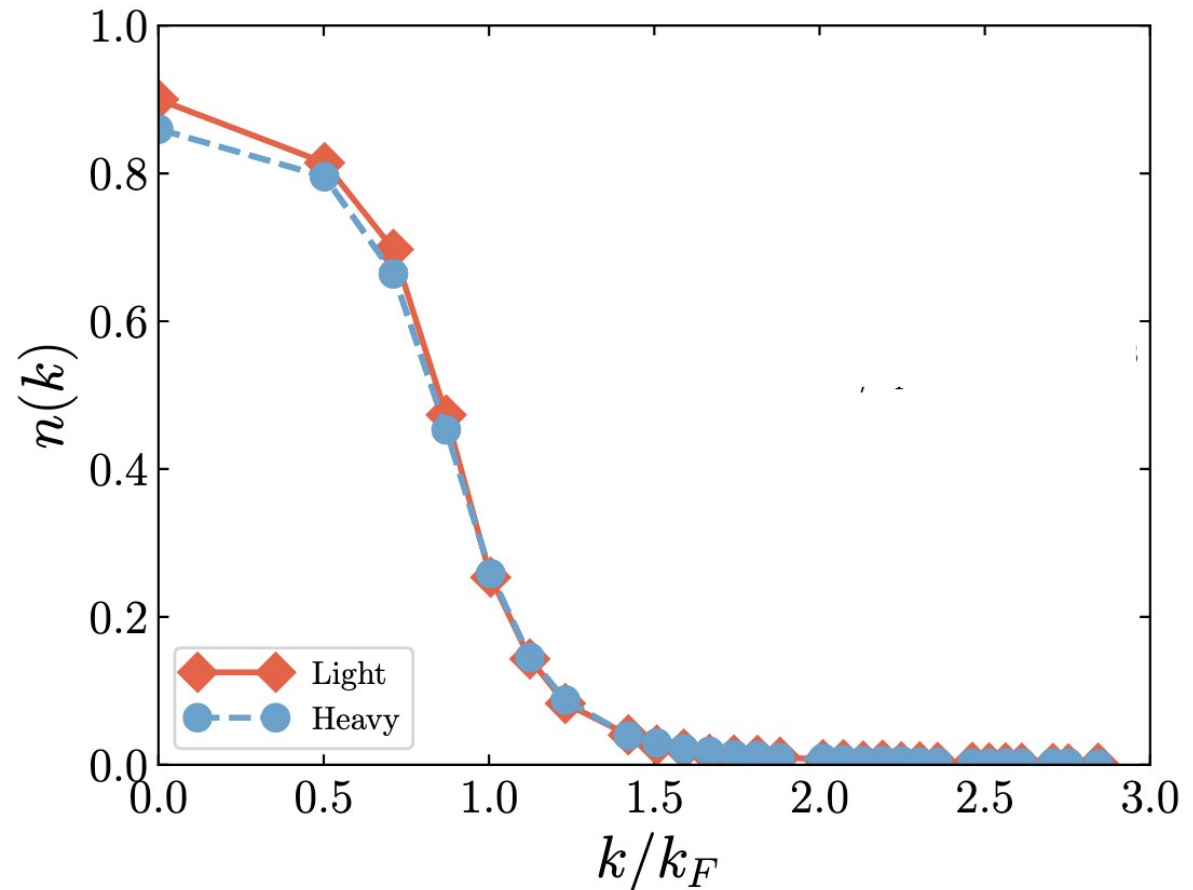
Equation of state



Mass imbalance

^6Li and ^{40}K
BCS-BEC crossover

Momentum
distribution

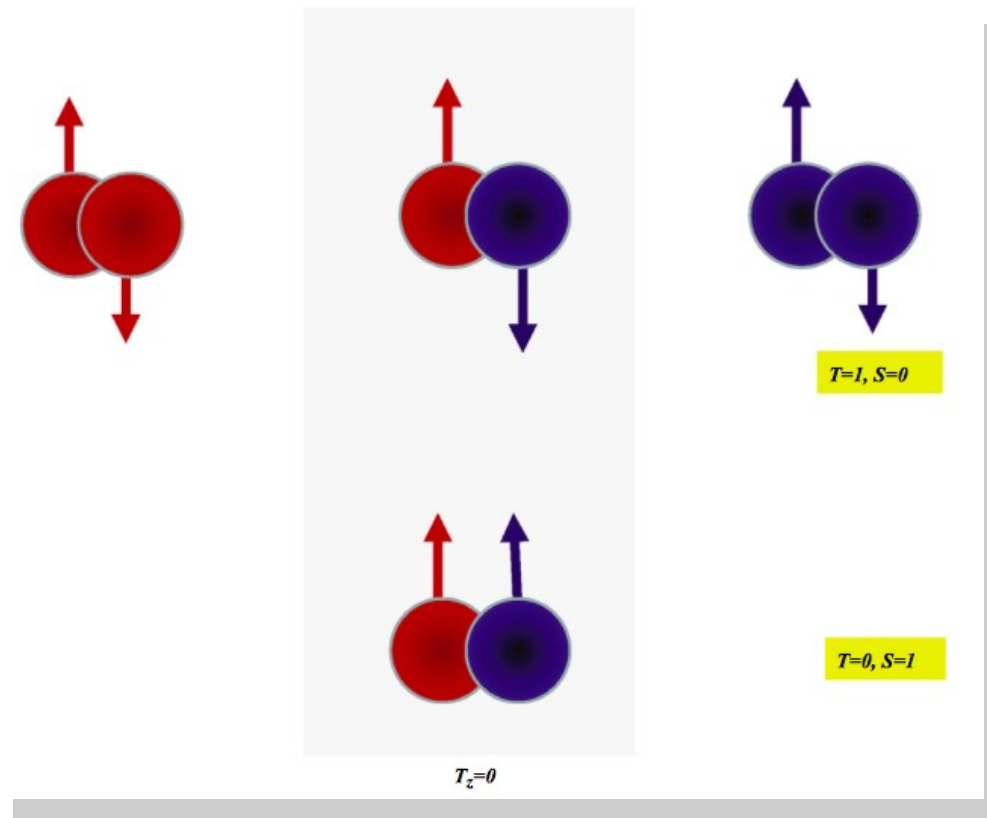


Four-component nucleons (in heavy nuclei)

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.

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 **81**, 064308 (2010)

Hamiltonian

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

- 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:

$$\rho = V^* V^T \quad \text{and} \quad \kappa = V^* U^T$$

- Hartree-Fock-Bogoliubov equations:

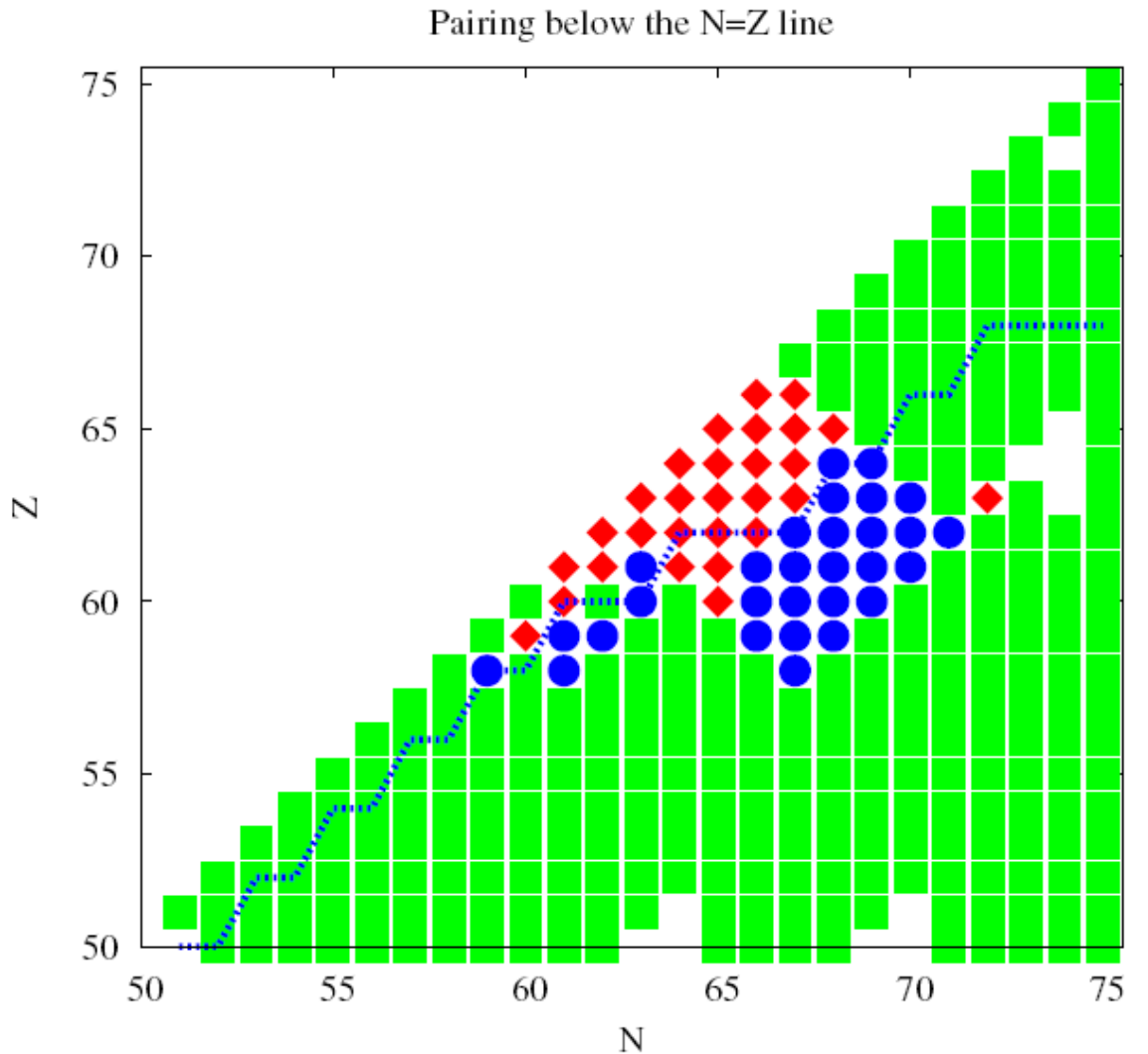
$$\begin{bmatrix} h' & \Delta \\ -\Delta^* & -h'^* \end{bmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = \begin{pmatrix} U_k \\ V_k \end{pmatrix} E_k$$

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

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

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

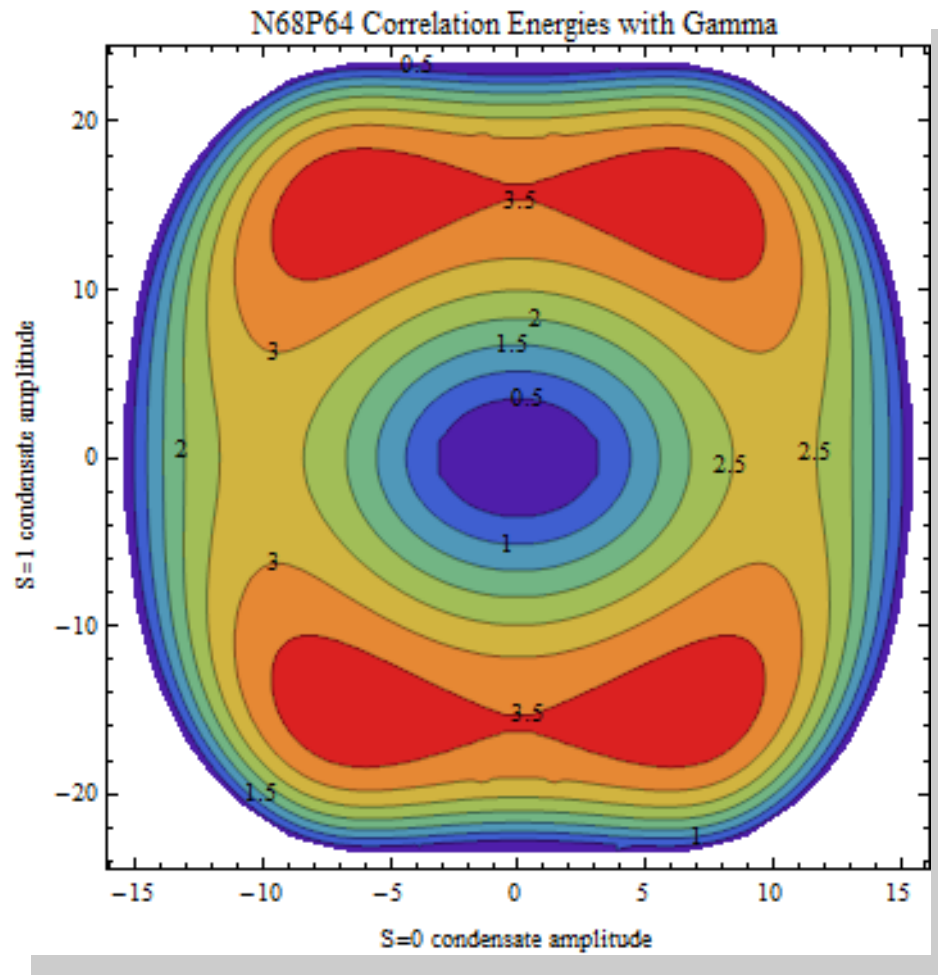
Pairing in heavy nuclei



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)

Energy contour for mixed spin



$$H^{00} = \text{Tr} \left(\varepsilon \rho + \frac{1}{2} \Gamma \rho - \frac{1}{2} \Delta \kappa^* \right)$$

- Fixed up Γ term (Hartree-Fock contribs)
- Effect weakened
- Note: still no deformation

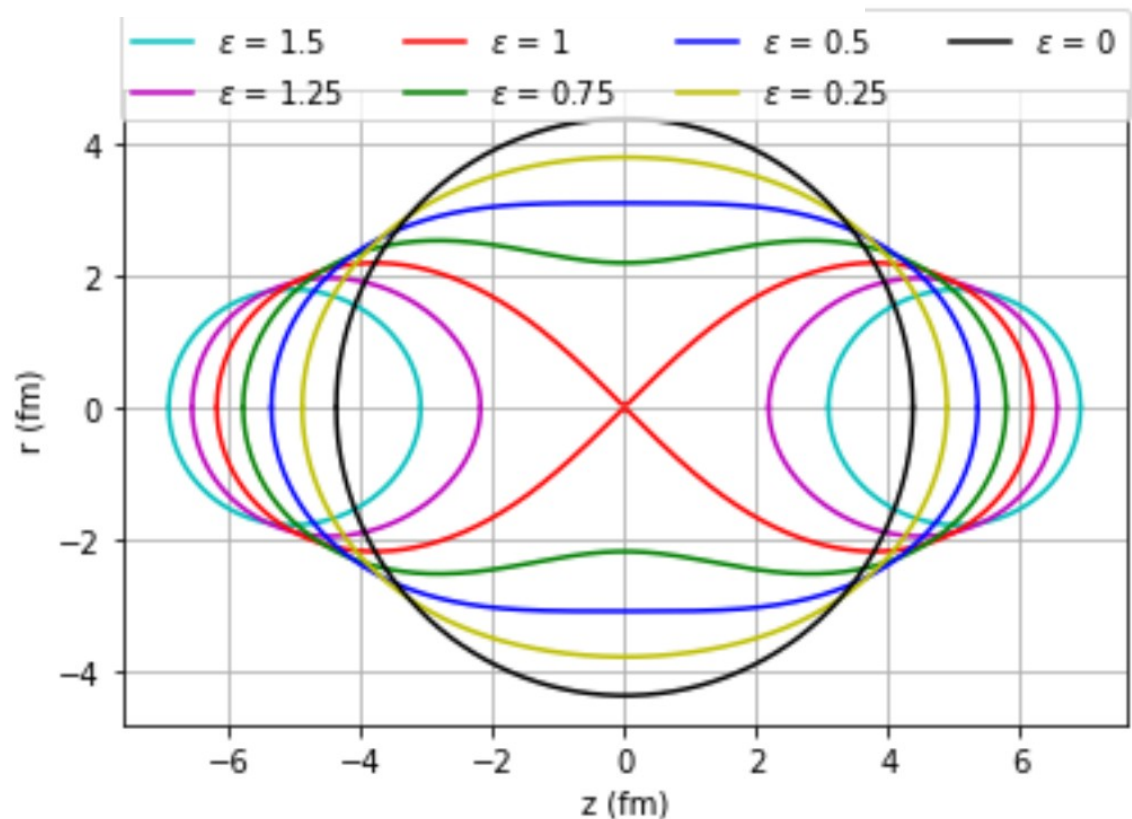
What about deformation?

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

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

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

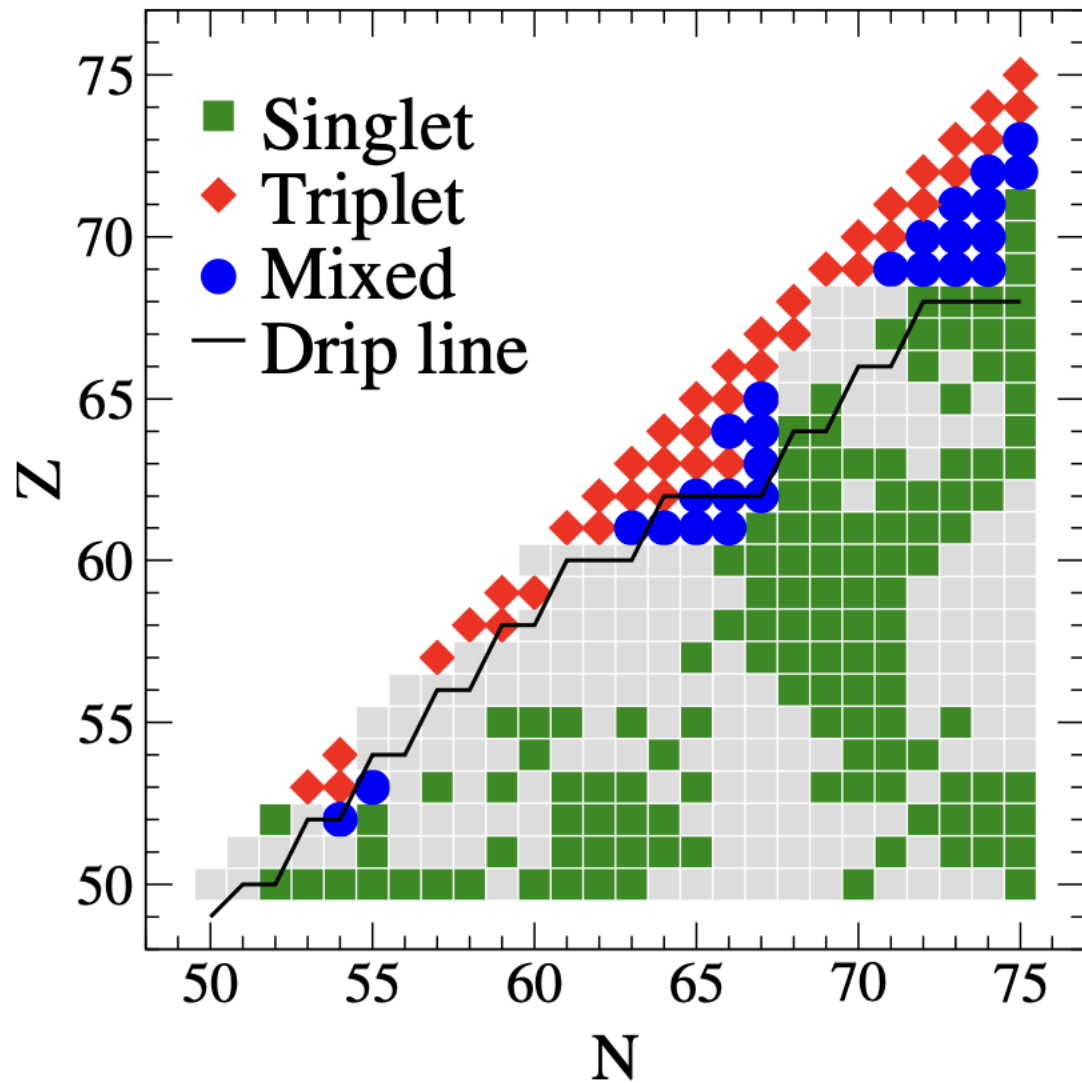
Surface is a
Cassini oval:



Deformation and exotic pairing

Deformation impacts
but does not kill
mixed-spin pairing:

- Quadrupole deformation is main factor
- For $N=Z$ deformation actually *enhances* spin-triplet pairing

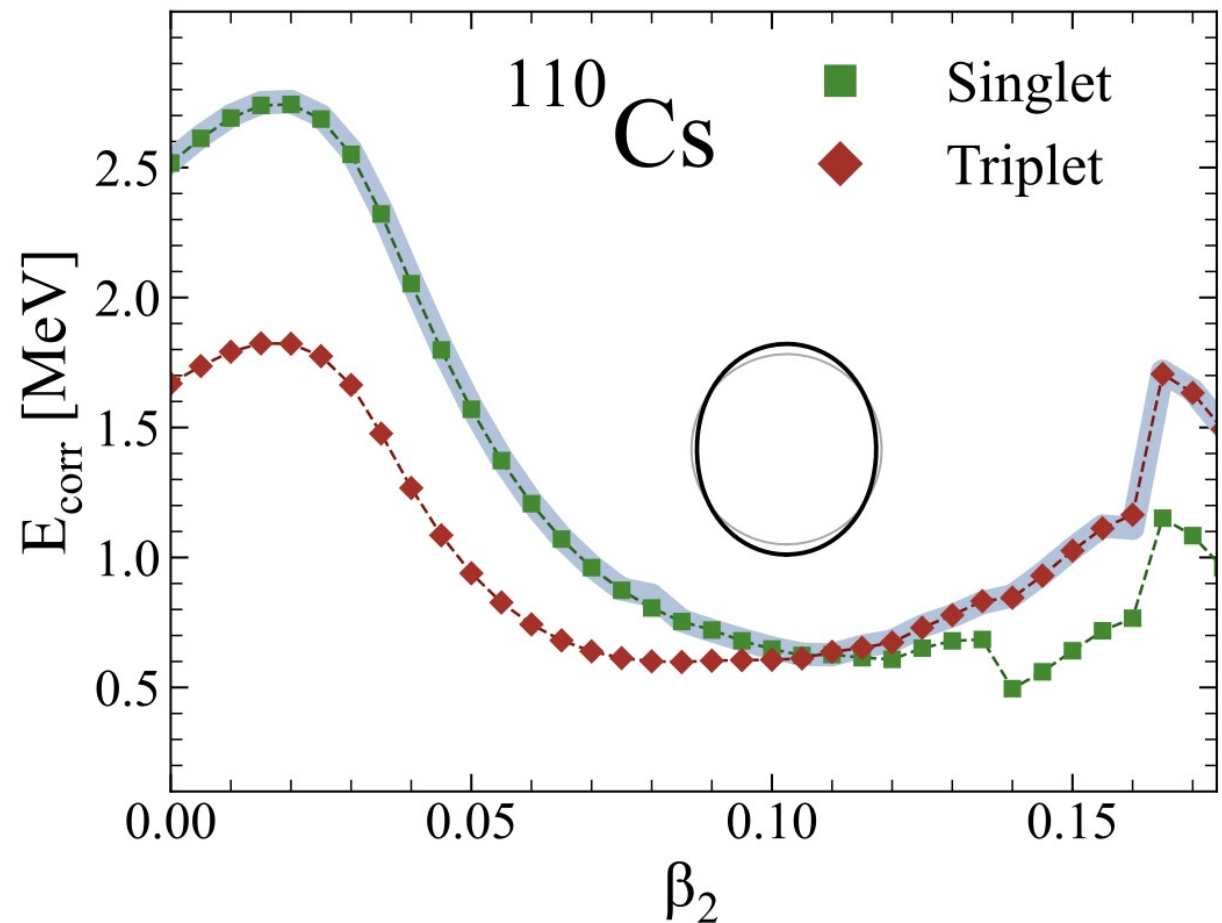


Deformation and exotic pairing

Vary quadrupole deformation and compare constrained with unconstrained runs.

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

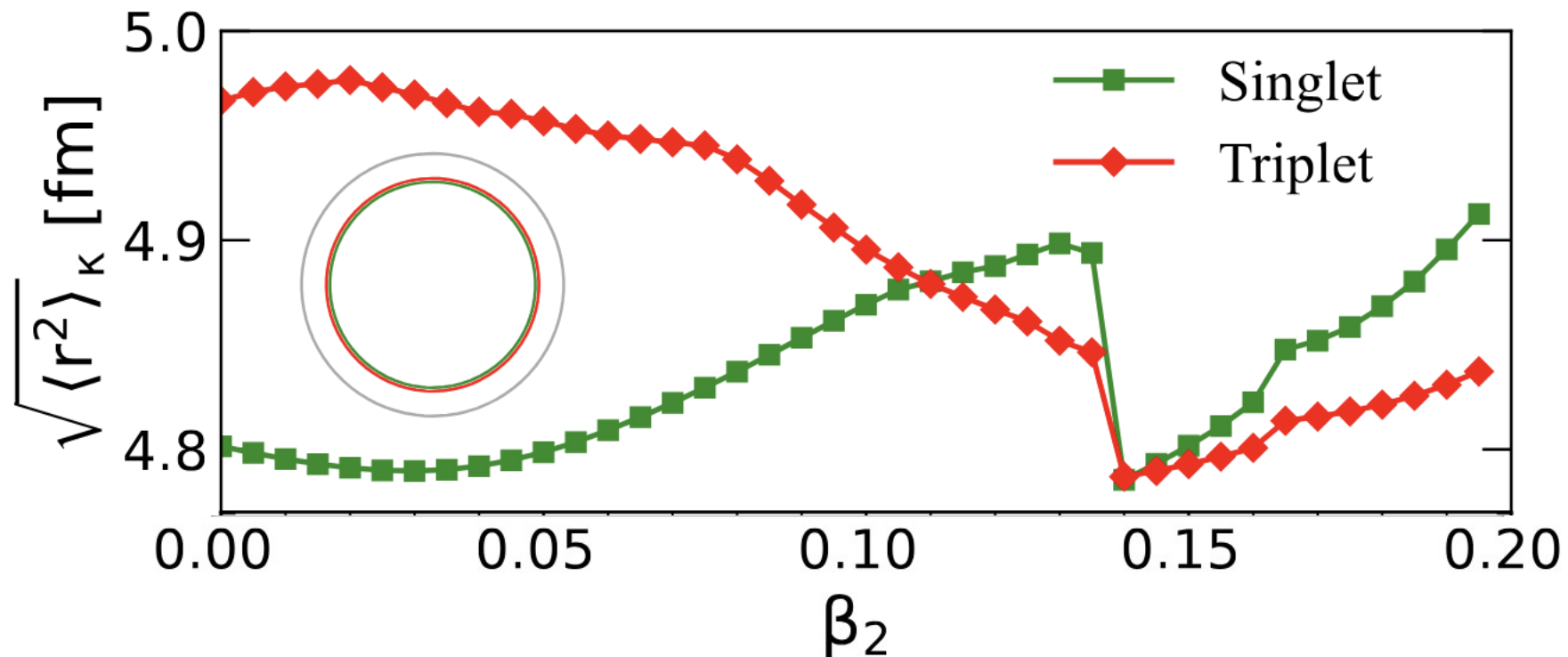
But spin-triplet pairs move to the interior of the nucleus and are unimpacted.



Deformation and exotic pairing

To see this explicitly:

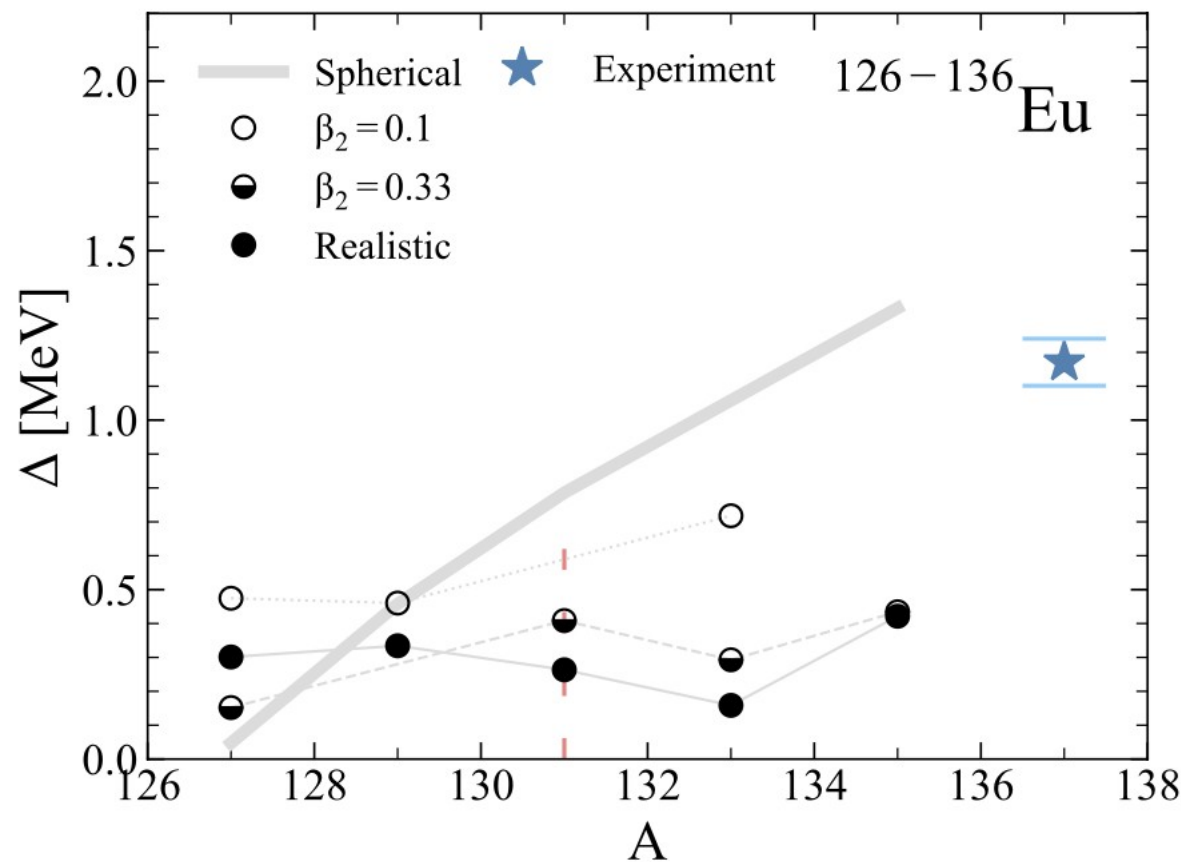
$$\sqrt{\langle r^2 \rangle_\kappa} = \left[\frac{\int d\rho dz (\rho^2 + z^2) \kappa^2(\rho, z)}{\int d\rho dz \kappa^2(\rho, z)} \right]^{1/2}$$
$$\kappa_\alpha(\rho, z) = \frac{1}{4\pi} \sum_{ij} u_i(\rho, z) u_j(\rho, z) \bar{A}_{\alpha, ij} \kappa_{ij}$$



Deformation and exotic pairing

Trying to connect with
experiment:

$$\Delta(n) = E_{\text{corr}}(n) - \frac{1}{2} [E_{\text{corr}}(n-1) + E_{\text{corr}}(n+1)]$$

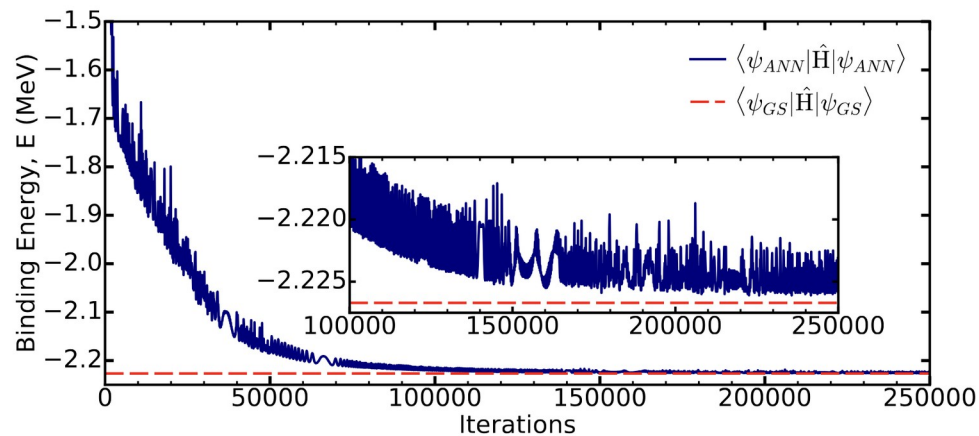


Neural-network wave functions for light nuclei (not really related to pairing)

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

Earlier work

Deuteron



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

Light nuclei

	Λ	VMC-ANN	VMC-JS	GFMC	GFMC _c
^2H	4 fm ⁻¹	-2.224(1)	-2.223(1)	-2.224(1)	-
	6 fm ⁻¹	-2.224(4)	-2.220(1)	-2.225(1)	-
^3H	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)
^4He	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

Spin-isospin correlations

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

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

for N2LO chiral Hamiltonian

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

Neural networks for light nuclei

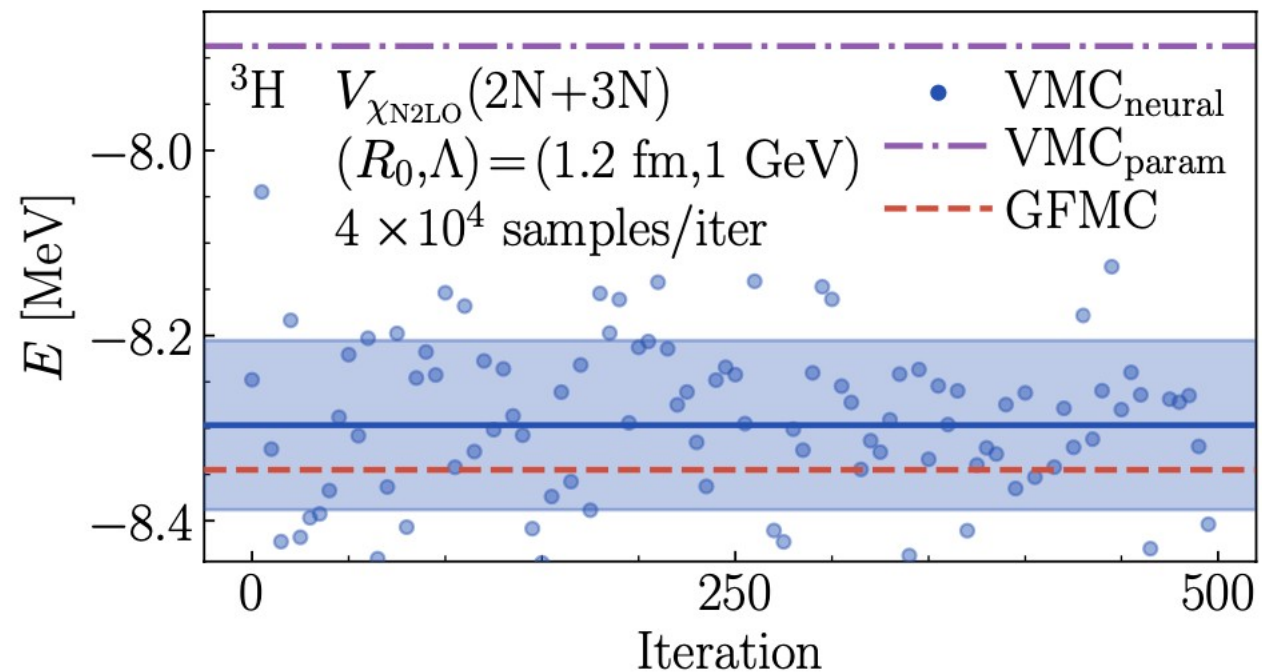
Nearly reproduces GFMC results
already at the VMC level

$E = E_k + V_{\chi\text{N}^2\text{LO}}(2\text{N})$				
	R_0 [fm]	E_{neural} [MeV]	E_{GFMC} [MeV]	$ \Delta E / E_{\text{GFMC}} $
${}^3\text{H}$	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%
${}^2\text{H}$	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

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



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

Conclusions

- 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

Takeaway

*Celuy qui n'avoit jamais veu de riviere,
à la premiere qu'il rencontra,
il pensa que ce fut l'Ocean.*

– Michel Eyquem de Montaigne
Essais, Livre I, Chapitre 27

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- Pengsheng Weng

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