From alpha clustering to homogeneous nucleonic matter

Alex Gezerlis

UNIVERSITY of GUELPH

Theory Canada 14
TRIUMF & UBC
May 31, 2019

Getting the TLAs out of the way

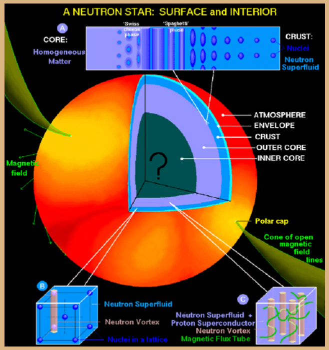
QCD = Quantum Chromodynamics

EFT = Effective Field Theory

QMC = Quantum Monte Carlo

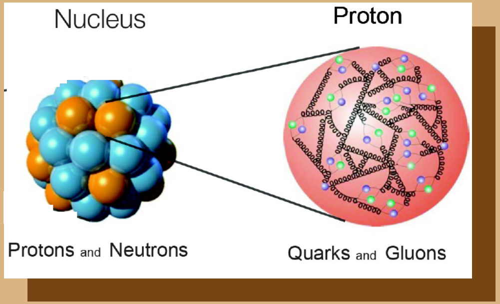
DFT = Density Functional Theory

Outline

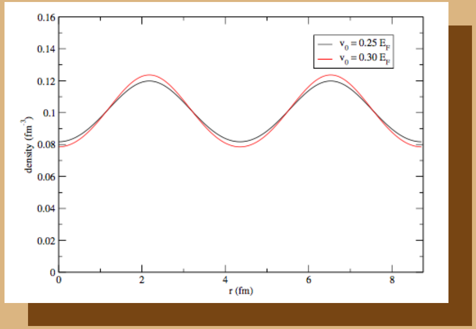


Credit: Dany Page

Motivation

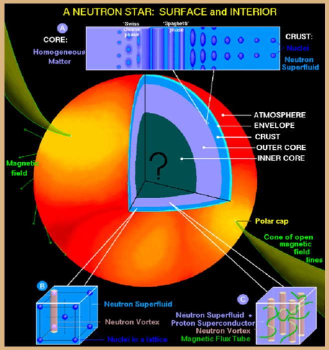


Nuclear background



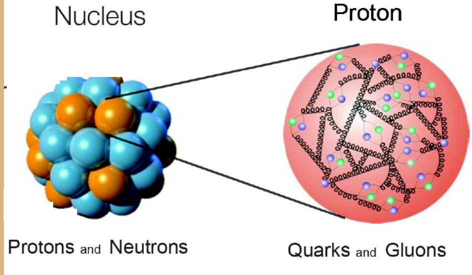
Recent results

Outline

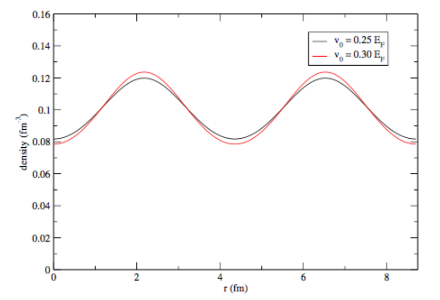


Credit: Dany Page

Motivation



Nuclear background



Recent results

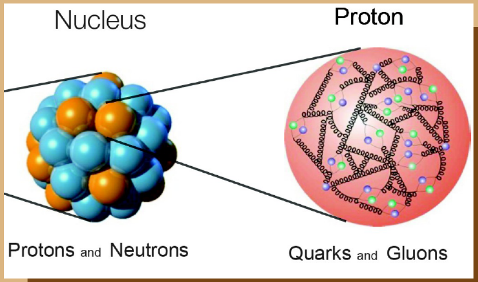
Key questions

1. What is the nature of the nuclear force that binds protons and neutrons into stable and rare isotopes?
2. What is the origin of simple patterns in complex nuclei?
3. How did visible matter come into being and how does it evolve?

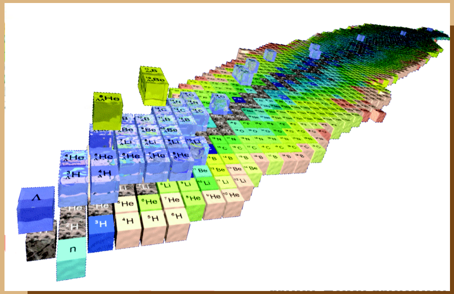
FRIB: Opening New Frontiers in Nuclear Science (2012), also LRP and NRC dec.

Physical systems studied

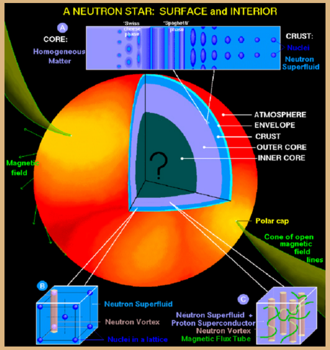
Nuclear forces



Nuclear structure

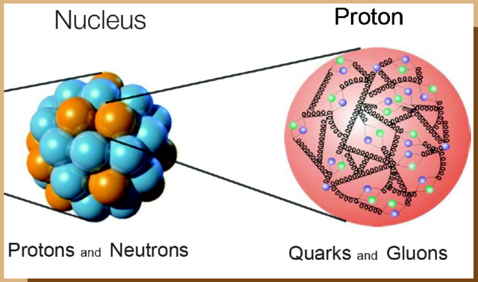


Nuclear astrophysics

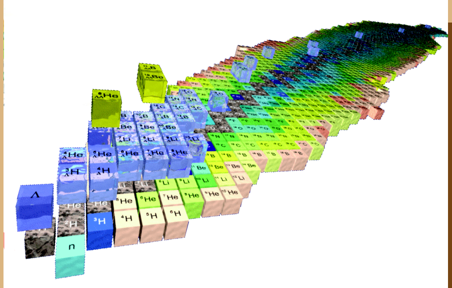


Physical systems studied

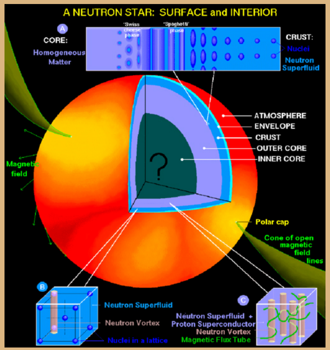
Nuclear forces

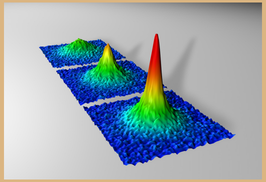


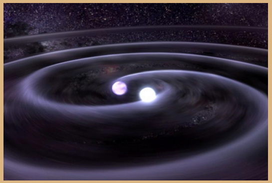
Nuclear structure



Nuclear astrophysics

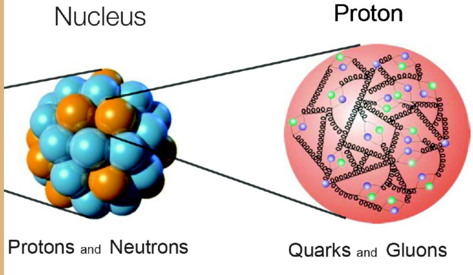




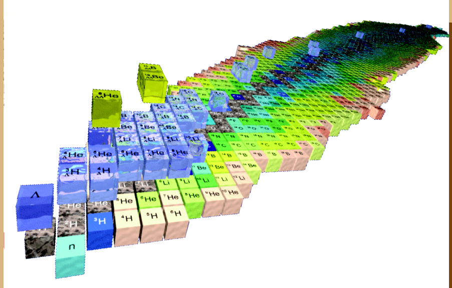


Physical systems studied

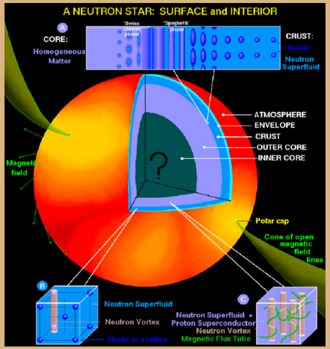
Few nucleons

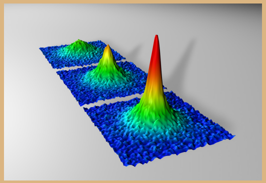


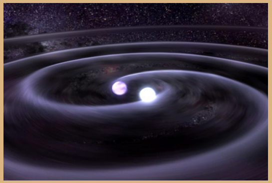
Many nucleons



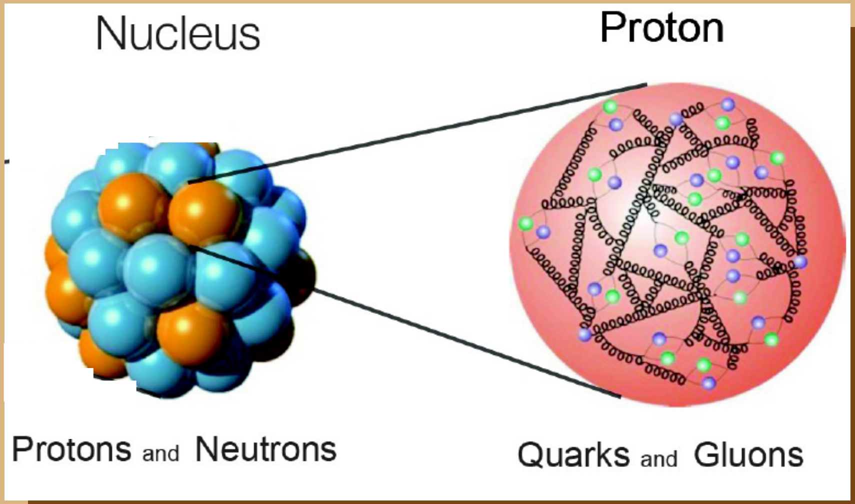
Very many nucleons





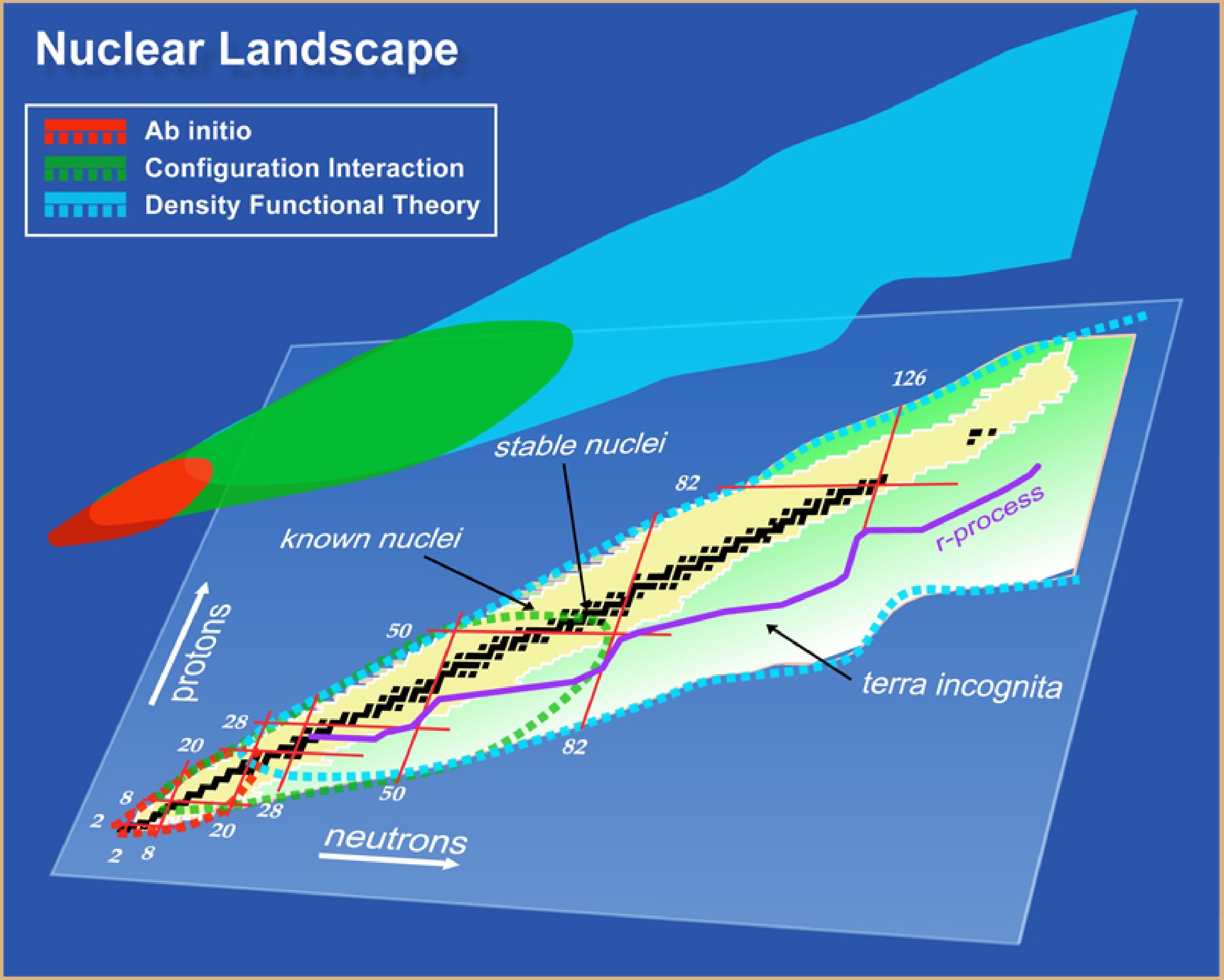


Key system: few nucleons



- 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

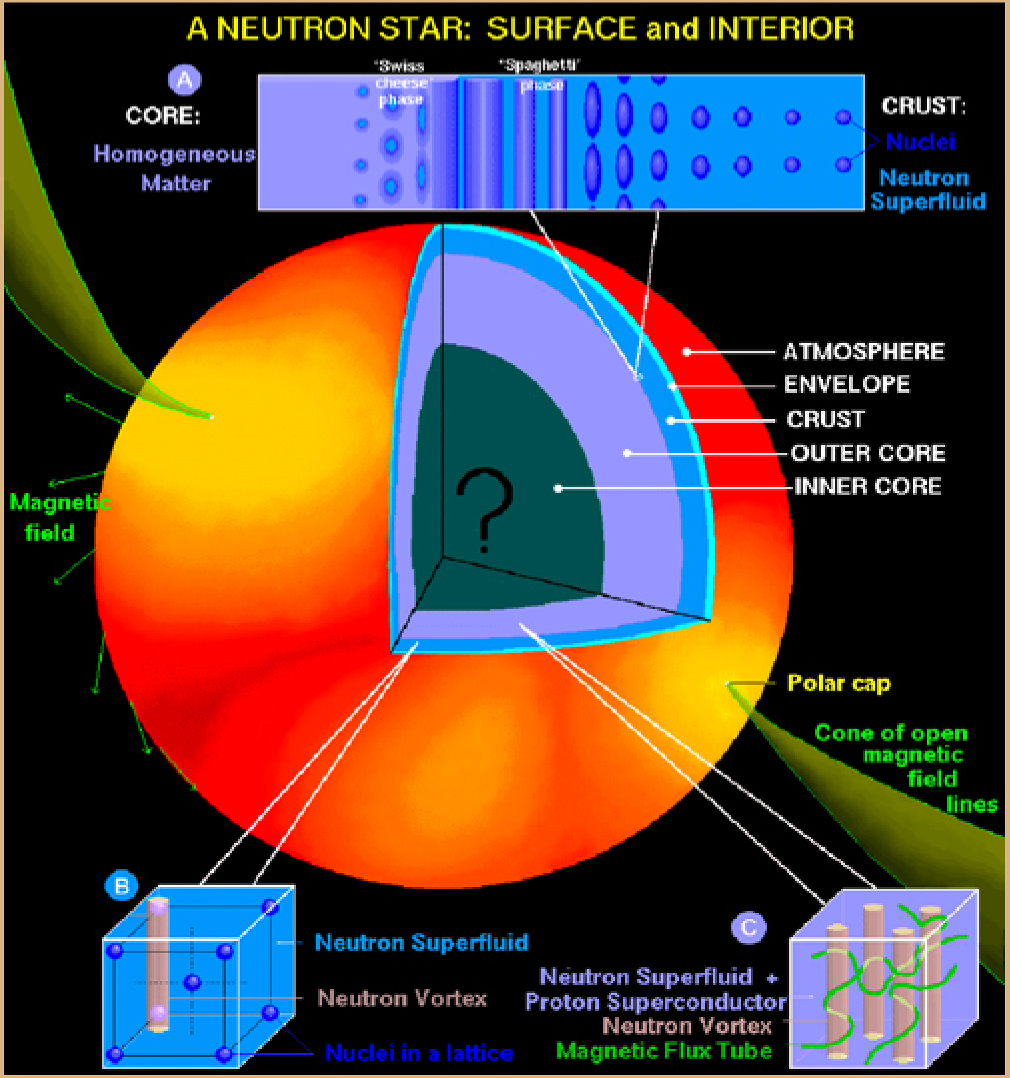
Key system: nuclei



- Experimental facilities continue to push the envelope
- Using complicated many-body methods we can try to "build nuclei from scratch"
- No universal theoretical method exists (yet?)
- Regions of overlap between different methods are crucial
- Goal is to study nuclei *from first principles* (when possible)

Key system: neutron stars

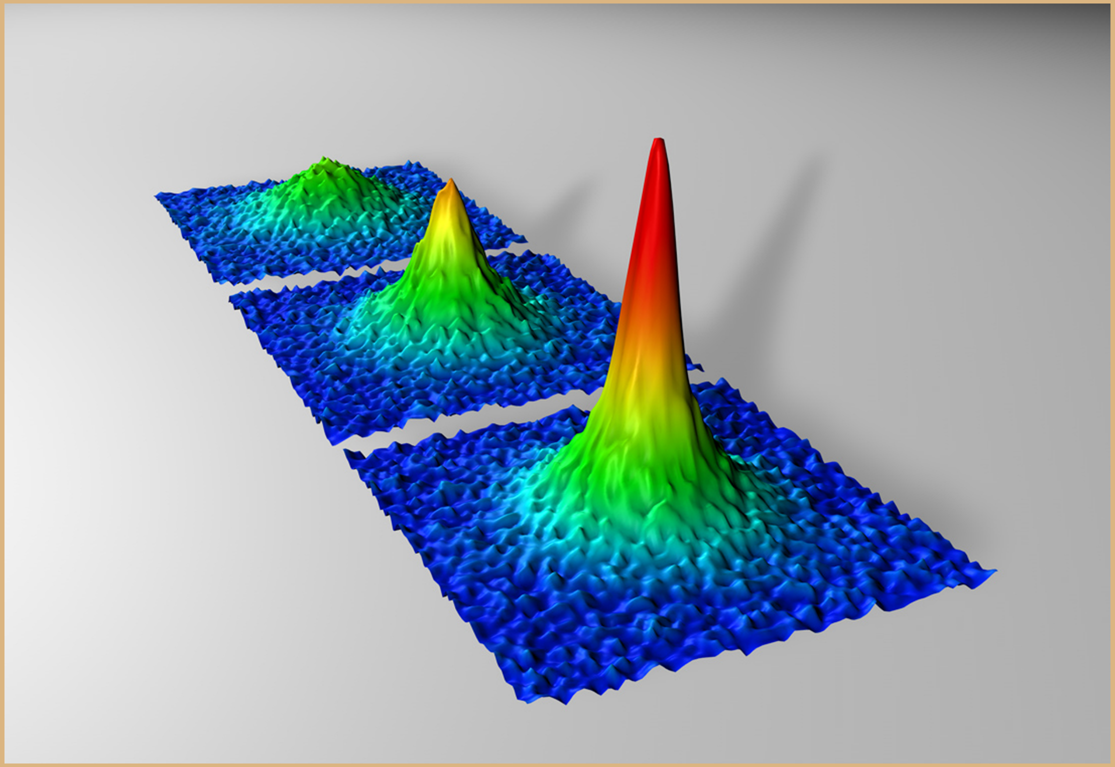
Neutron stars as ultra-dense matter laboratories



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)

Key system: cold atoms

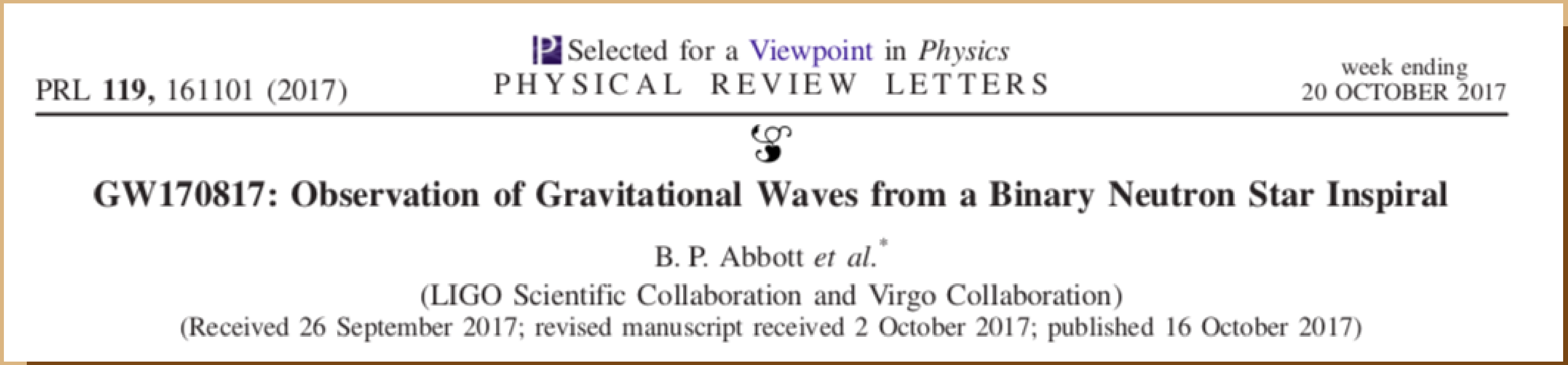


Credit: University of Colorado

- Starting in the 1990s, it became possible to experimentally probe degenerate bosonic atoms (beyond ^{4}He)
- Starting in the 2000s, the same happened for fermionic atoms (beyond ^{3}He)
- 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

Key system: binaries

Credit: LIGO first detection PRL



Selected for a Viewpoint in *Physics*

PRL **119,** 161101 (2017) PHYSICAL REVIEW LETTERS week ending 20 OCTOBER 2017

GW170817: Observation of Gravitational Waves from a Binary Neutron Star Inspiral

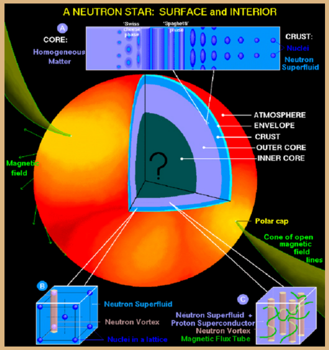
B. P. Abbott *et al.**

(LIGO Scientific Collaboration and Virgo Collaboration)

(Received 26 September 2017; revised manuscript received 2 October 2017; published 16 October 2017)

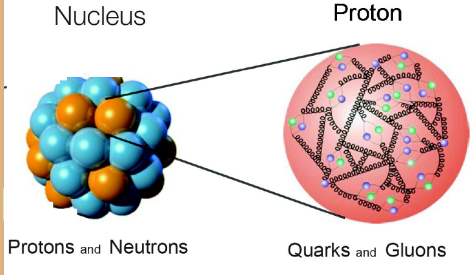
- New era of gravitational wave astronomy (more like a microphone than a telescope)
- Several black-hole binary detections, a NS-NS event, and many rumors

Outline

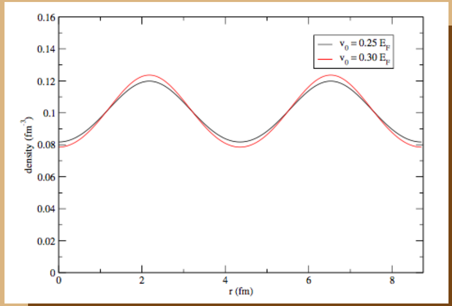


Credit: Dany Page

Motivation



Nuclear background



Recent results

Nuclear interactions 1

Historically

“Effective Interactions” were employed in the context of mean-field theory.

Phenomenological

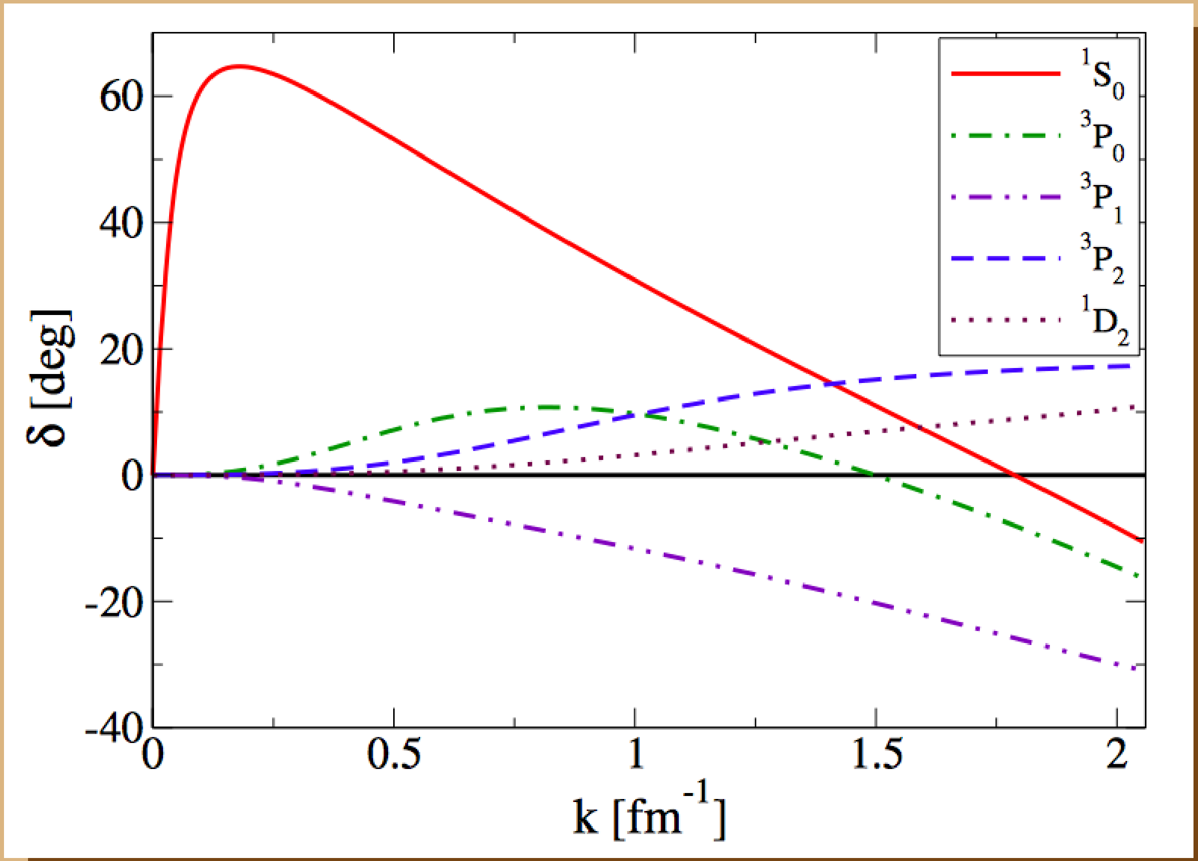
NN interaction fit to N-body experiment

Non-microscopic

NN interaction does not claim to (and will not) describe np scattering

Nuclear physics is difficult

Scattering phase shifts: different “channels” have different behavior.



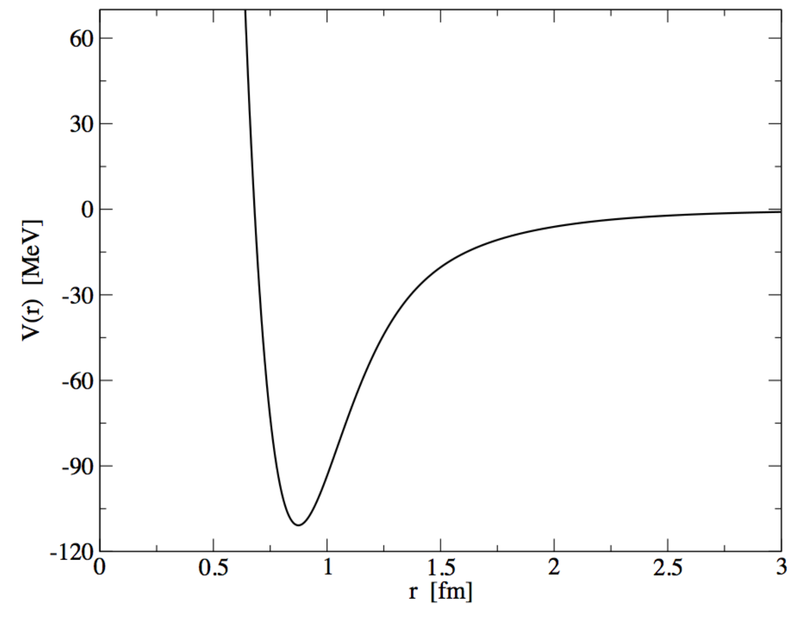
Any potential that reproduces them must be spin (and isospin) dependent

Nuclear interactions 2

Different approach: phenomenology treats NN scattering without connecting with the underlying level

$$V_2 = \sum_{j<k} v_{jk} = \sum_{j<k} \sum_{p=1}^{8} v_p(r_{jk}) O^{(p)}(j,k)$$

$$O^{p=1,8}(j,k) = (1, \sigma_j \cdot \sigma_k, S_{jk}, \mathbf{L}_{jk} \cdot \mathbf{S}_{jk}) \otimes (1, \tau_j \cdot \tau_k)$$



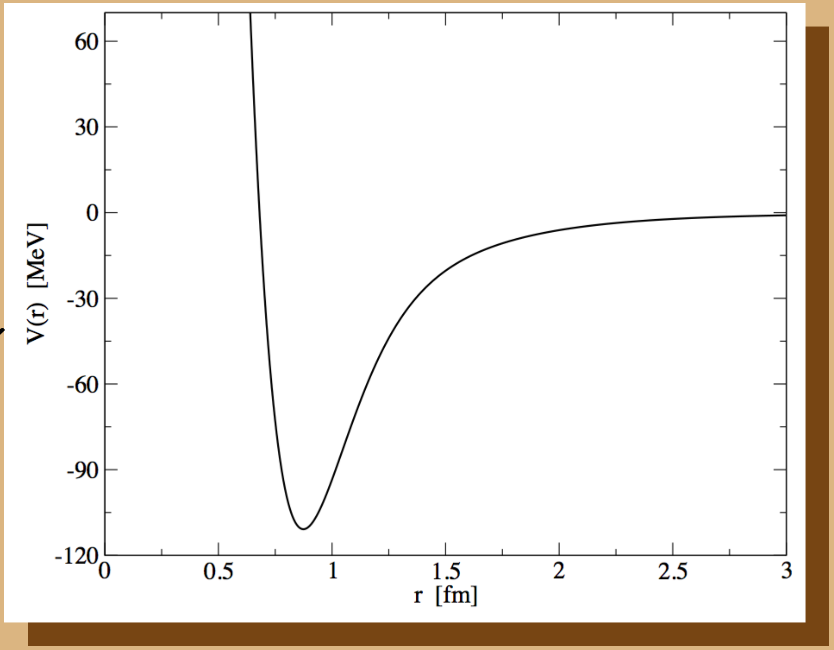
Nuclear interactions 2

Different approach: phenomenology treats NN scattering without connecting with the underlying level

$$V_2 = \sum_{j<k} v_{jk} = \sum_{j<k} \sum_{p=1}^{8} v_p(r_{jk}) O^{(p)}(j,k)$$

$$O^{p=1,8}(j,k) = (1, \sigma_j \cdot \sigma_k, S_{jk}, \mathbf{L}_{jk} \cdot \mathbf{S}_{jk}) \otimes (1, \tau_j \cdot \tau_k)$$

Such potentials are hard, making them non-perturbative at the many-body level (which is a problem for most methods on the market).



Softer, momentum-space formulations like CD-Bonn very popular

How to go beyond?

Historically, fit NN interaction to N-body experiment

Parallel approach, fit NN interaction to 2-body experiment, ignoring underlying level of quarks and gluons

How to go beyond?

Historically, fit NN interaction to N-body experiment

Parallel approach, fit NN interaction to 2-body experiment, ignoring underlying level of quarks and gluons

Natural goal: fit NN interaction to 2-body experiment,
without ignoring underlying level

Chiral effective field theory

Nuclear Hamiltonian: chiral EFT

How to build on QCD in a systematic manner?

Exploit separation of scales:

$$a_{^1S_0} = (11\ \mathrm{MeV})^{-1}$$

$$m_\pi = 140\ \mathrm{MeV}$$

$$\Lambda_\chi \approx m_\rho \approx\ 800\ \mathrm{MeV}$$

Nuclear Hamiltonian: chiral EFT

How to build on QCD in a systematic manner?

Exploit separation of scales: $a_{^1S_0} = (11\ \mathrm{MeV})^{-1}$

$m_\pi = 140\ \mathrm{MeV}$

$\Lambda_\chi \approx m_\rho \approx\ 800\ \mathrm{MeV}$

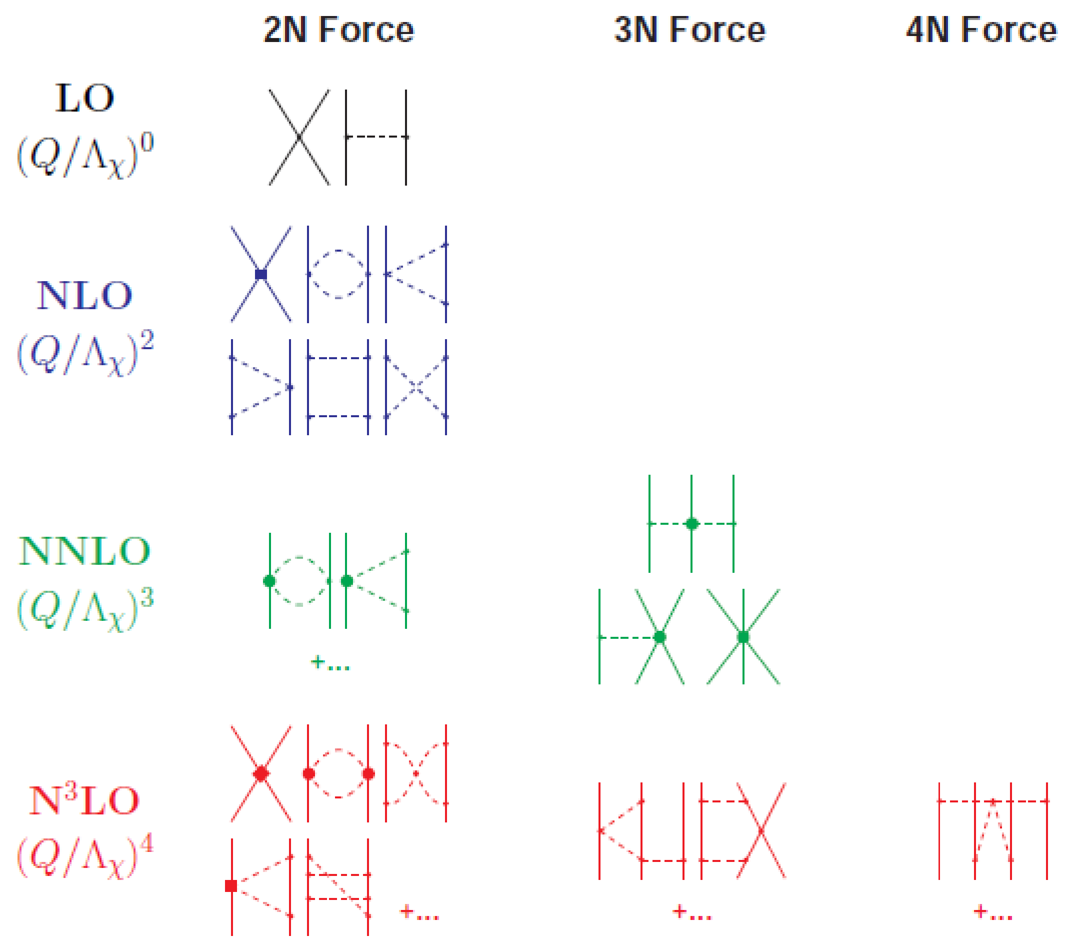
Chiral Effective Field Theory approach:

Use nucleons and pions as degrees of freedom

Systematically expand in $\frac{Q}{\Lambda_\chi}$

Program introduced by S. Weinberg, now taken over by the nuclear community

Nuclear interactions 3



- Attempts to connect with underlying theory (QCD)
- Systematic low-momentum expansion
- Consistent many-body forces
- Low-energy constants from experiment or lattice QCD
- Until recently non-local in coordinate space, so unused in continuum QMC
- Power counting's relation to renormalization still an open question

What is more

Successful nuclear QMC program constrained to use local potentials as input.

What does “local” mean?

In particle physics: potential is defined at one point in space-time (contact)

In nuclear physics:

$$\langle \mathbf{r}' | \hat{V} | \mathbf{r} \rangle = \begin{cases} V(\mathbf{r})\ \delta^3(\mathbf{r}' - \mathbf{r}) & \text{if local.} \\ V(\mathbf{r}', \mathbf{r}) & \text{if nonlocal.} \end{cases}$$

which is equivalent to

$$\langle \mathbf{p}' | \hat{V} | \mathbf{p} \rangle = \begin{cases} V(\mathbf{p}' - \mathbf{p}) & \text{if local.} \\ V(\mathbf{p}', \mathbf{p}) & \text{if nonlocal.} \end{cases}$$

Nuclear forces: summary

Local high-quality phenomenology is hard

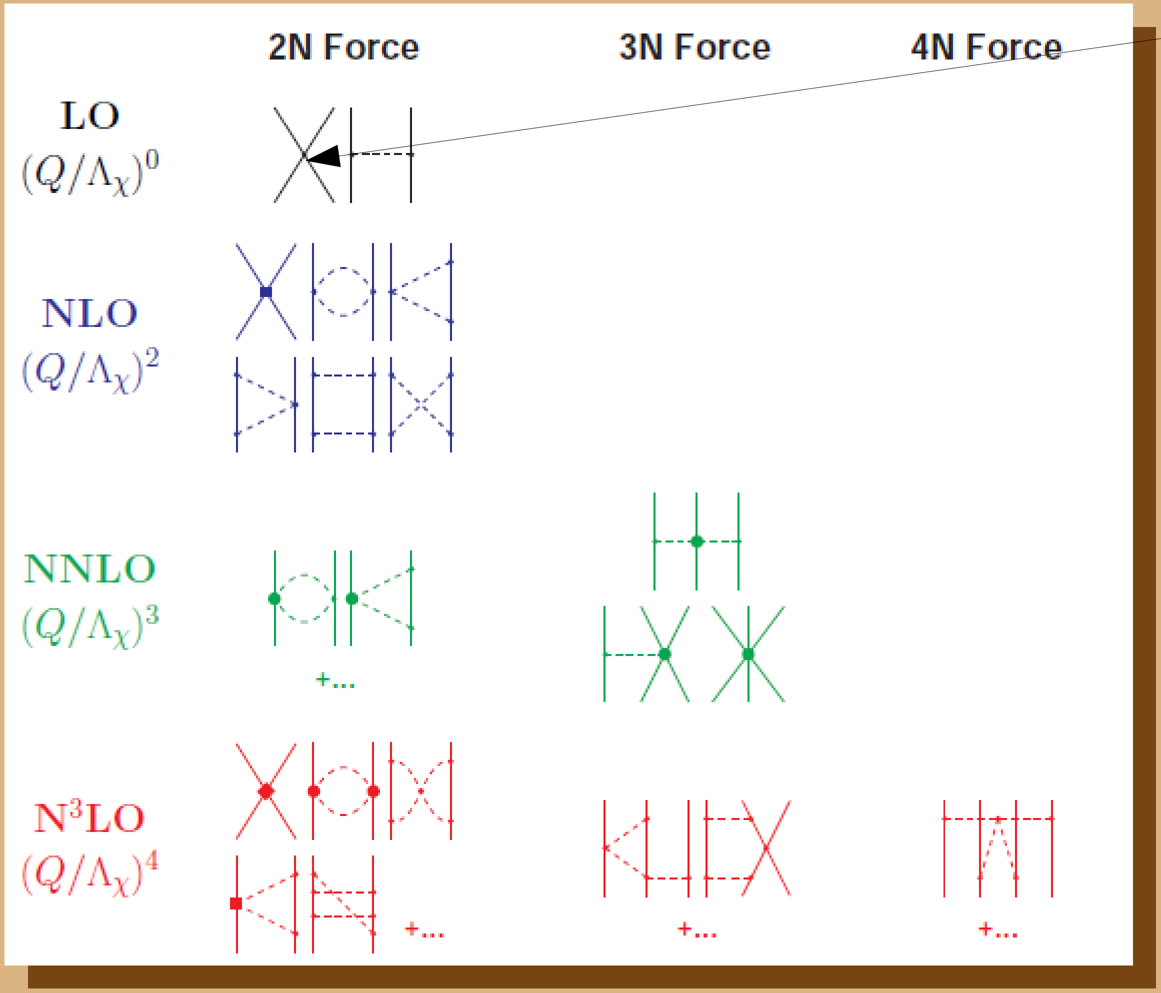
Consubstantial with the successes of nuclear QMC,
difficult to use in most other many-body methods

Chiral EFT
a) is connected to symmetries of QCD
b) has consistent many-body forces, and
c) allows us to produce systematic uncertainty bands
also happened to be non-local (such are the *sumbebekota*)

Heavily used in other methods, but previously not used in nuclear QMC

Turning to the resolution

Nuclear Hamiltonian: chiral EFT



$$V_{\mathrm{ct}}^{(0)} = C_S + C_T \; \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$$

Merely the standard choice.

Actually 4 terms in full set
consistent with the symmetries of QCD

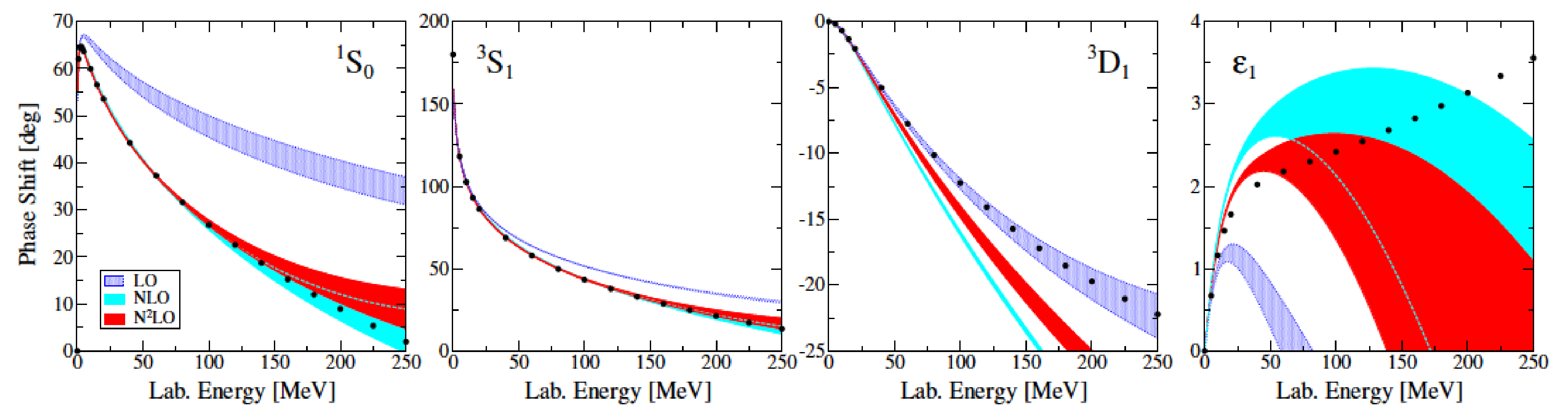
$$\begin{aligned} V_{\mathrm{ct}}^{(0)} &= C_1 + C_2 \; \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \\ &+ C_3 \; \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 + C_4 \; \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \; \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \end{aligned}$$

Pick 2 and antisymmetrize

A. Gezerlis, I. Tews, E. Epelbaum, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, Phys. Rev. Lett. **111**, 032501 (2013).

A. Gezerlis, I. Tews, E. Epelbaum, M. Freunek, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, Phys. Rev. C **90**, 054323 (2014).

Local chiral EFT



A. Gezerlis, I. Tews, E. Epelbaum, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, Phys. Rev. Lett. **111**, 032501 (2013).

A. Gezerlis, I. Tews, E. Epelbaum, M. Freunek, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, Phys. Rev. C **90**, 054323 (2014).

J. E. Lynn, J. Carlson, E. Epelbaum, S. Gandolfi, **A. Gezerlis**, K. E. Schmidt, A. Schwenk, I. Tews, Phys. Rev. Lett. **113**, 192501 (2014)

I. Tews, S. Gandolfi, **A. Gezerlis**, A. Schwenk, Phys. Rev. C **93**, 024305 (2016)

J. E. Lynn, I. Tews, J. Carlson, S. Gandolfi, **A. Gezerlis**, K. E. Schmidt, A. Schwenk, I. Tews, Phys. Rev. Lett. **116**, 062501 (2016)

P. Klos, J. E. Lynn, I. Tews, S. Gandolfi, **A. Gezerlis**, H.-W. Hammer, and A. Schwenk, Phys. Rev. C, **94**, 054005 (2017)

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

Nuclear many-body problem

$$H\Psi = E\Psi$$

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

so

$$H\Psi(\mathbf{r}_1, \cdots, \mathbf{r}_A; s_1, \cdots, s_A; t_1, \cdots, t_A) = E\Psi(\mathbf{r}_1, \cdots, \mathbf{r}_A; s_1, \cdots, s_A; t_1, \cdots, t_A)$$

i.e. $2^A \binom{A}{Z}$ complex coupled second-order differential equations

Nuclear many-body methods

Phenomenological (fit to A-body experiment)

Ab initio (fit to few-body experiment)

Nuclear many-body methods

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

Nuclear many-body methods

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

Main many-body methods employed (by me)

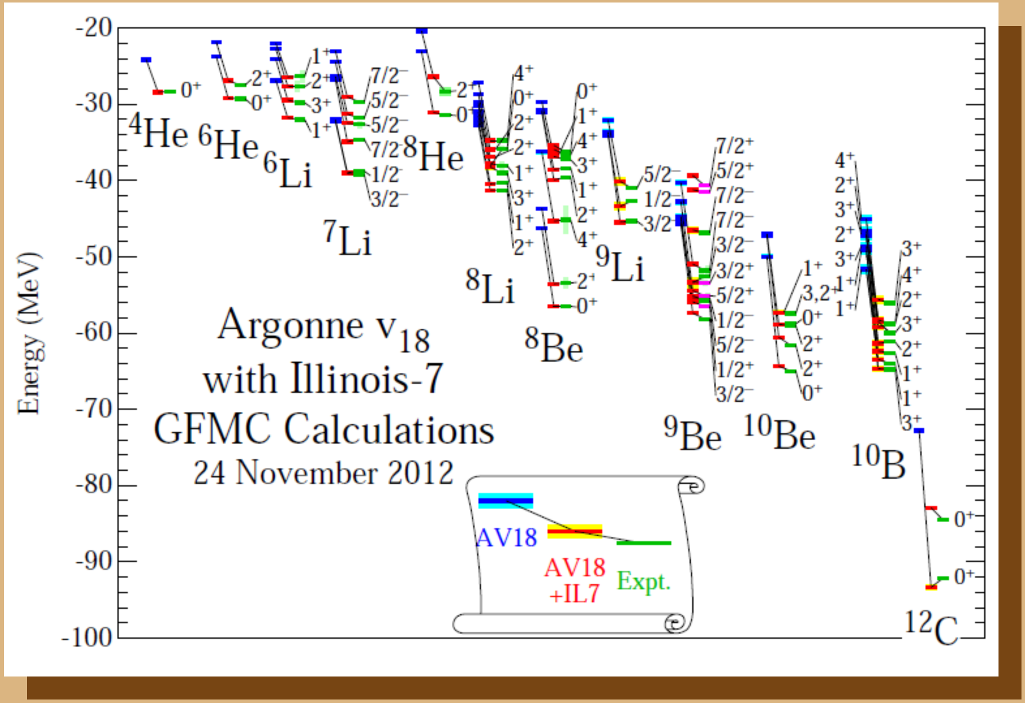
Two complementary methods

Quantum Monte Carlo

- Microscopic
- Computationally demanding (3N particle coordinates + spins)
- Limited to smallish N

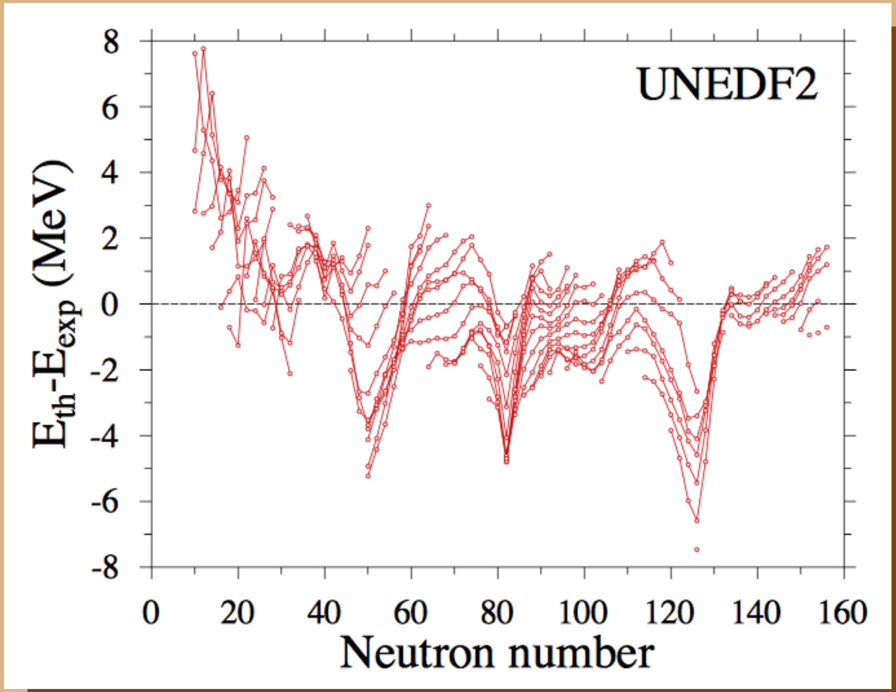
$$\Psi(\tau \to \infty) = \lim_{\tau \to \infty} e^{-(\mathcal{H}-E_T)\tau} \Psi_V$$

$$\to \alpha_0 e^{-(E_0-E_T)\tau} \Psi_0$$



Credit: Steve Pieper

Two complementary methods



Credit: W. Nazarewicz

Density Functional Theory

- More phenomenological (to date, but see major developments)
- Easier in crude form (orbitals → density → energy density)
- Can do any large N

$$E = \int d^3r \, \{\mathcal{E}[\rho(\mathbf{r})] + \rho(\mathbf{r})V_{\text{ext}}(\mathbf{r})\}$$

Two complementary methods

Quantum Monte Carlo

- Microscopic
- Computationally demanding (3N particle coordinates + spins)
- Limited to smallish N

$$\Psi(\tau \to \infty) = \lim_{\tau \to \infty} e^{-(\mathcal{H}-E_T)\tau}\Psi_V$$

$$\to \alpha_0 e^{-(E_0-E_T)\tau}\Psi_0$$

Density Functional Theory

- More phenomenological (to date, but see major developments)
- Easier in crude form (orbitals → density → energy density)
- Can do any large N

$$E = \int d^3r \, \{\mathcal{E}[\rho(\mathbf{r})] + \rho(\mathbf{r})V_{\mathrm{ext}}(\mathbf{r})\}$$

Two complementary methods

Quantum Monte Carlo

- Microscopic
- Computationally demanding (3N particle coordinates + spins)
- Limited to smallish N

$$\Psi(\tau \to \infty) = \lim_{\tau \to \infty} e^{-(\mathcal{H}-E_T)\tau}\Psi_V$$
$$\to \alpha_0 e^{-(E_0-E_T)\tau}\Psi_0$$

Density Functional Theory

- More phenomenological (to date, but see major developments)
- Easier in crude form (orbitals → density → energy density)
- Can do any large N

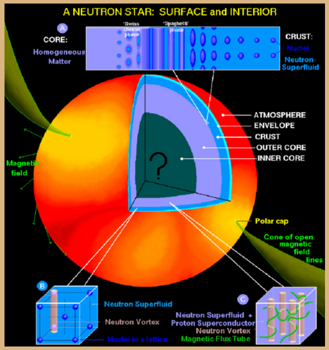
$$E = \int d^3r\,\{\mathcal{E}[\rho(\mathbf{r})] + \rho(\mathbf{r})V_{\text{ext}}(\mathbf{r})\}$$

Research Strategies

i) Use QMC as a benchmark with which to compare DFT results

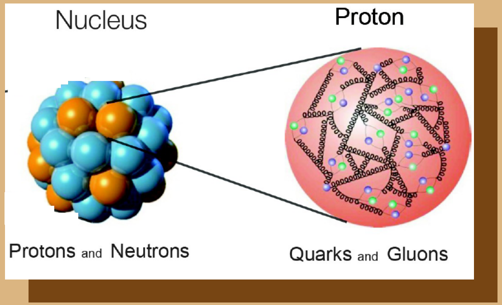
ii) Constrain DFT with QMC, then use DFT to make predictions

Outline

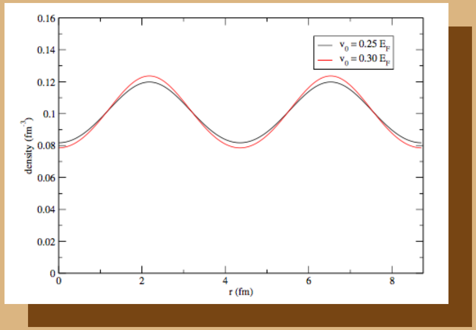


Credit: Dany Page

Motivation



Nuclear background



Recent results

From few to many: a selection

Connection with cold-atom experiment

Alpha clustering

Effective mass extraction

1. Connection with cold-atom experiment

Coupling

Weak coupling

- $k_F a \to 0$
- Studied for decades
- Experimentally difficult
- Pairing exponentially small
- Analytically known

Strong Coupling

- $k_F a \to \infty$
- More recent (2000s)
- Experimentally probed
- Pairing significant
- Non-perturbative

Coupling

Weak coupling

- $k_F a \to 0$
- Studied for decades
- Experimentally difficult
- Pairing exponentially small
- Analytically known

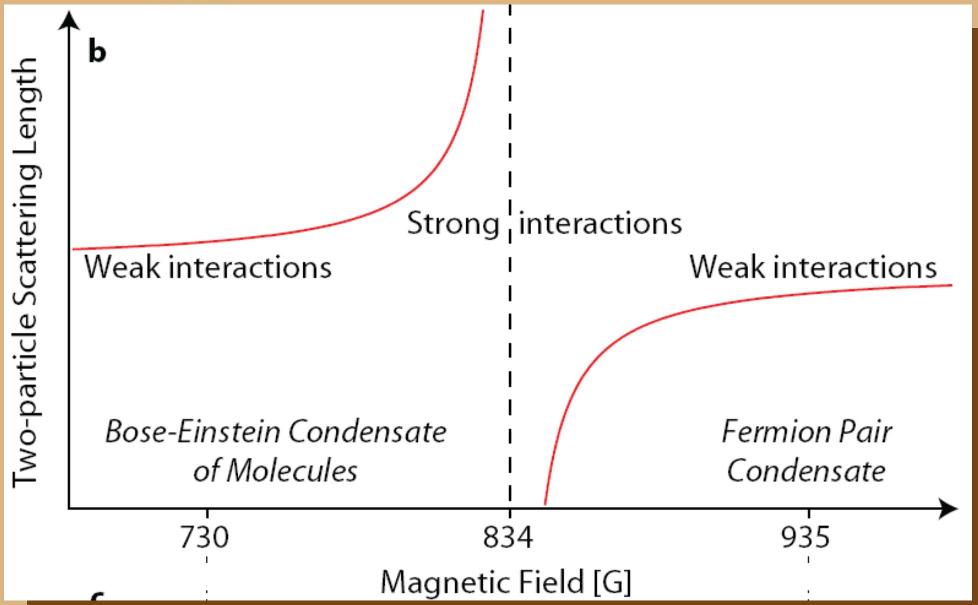
Strong Coupling

- $k_F a \to \infty$
- More recent (2000s)
- Experimentally probed
- Pairing significant
- Non-perturbative

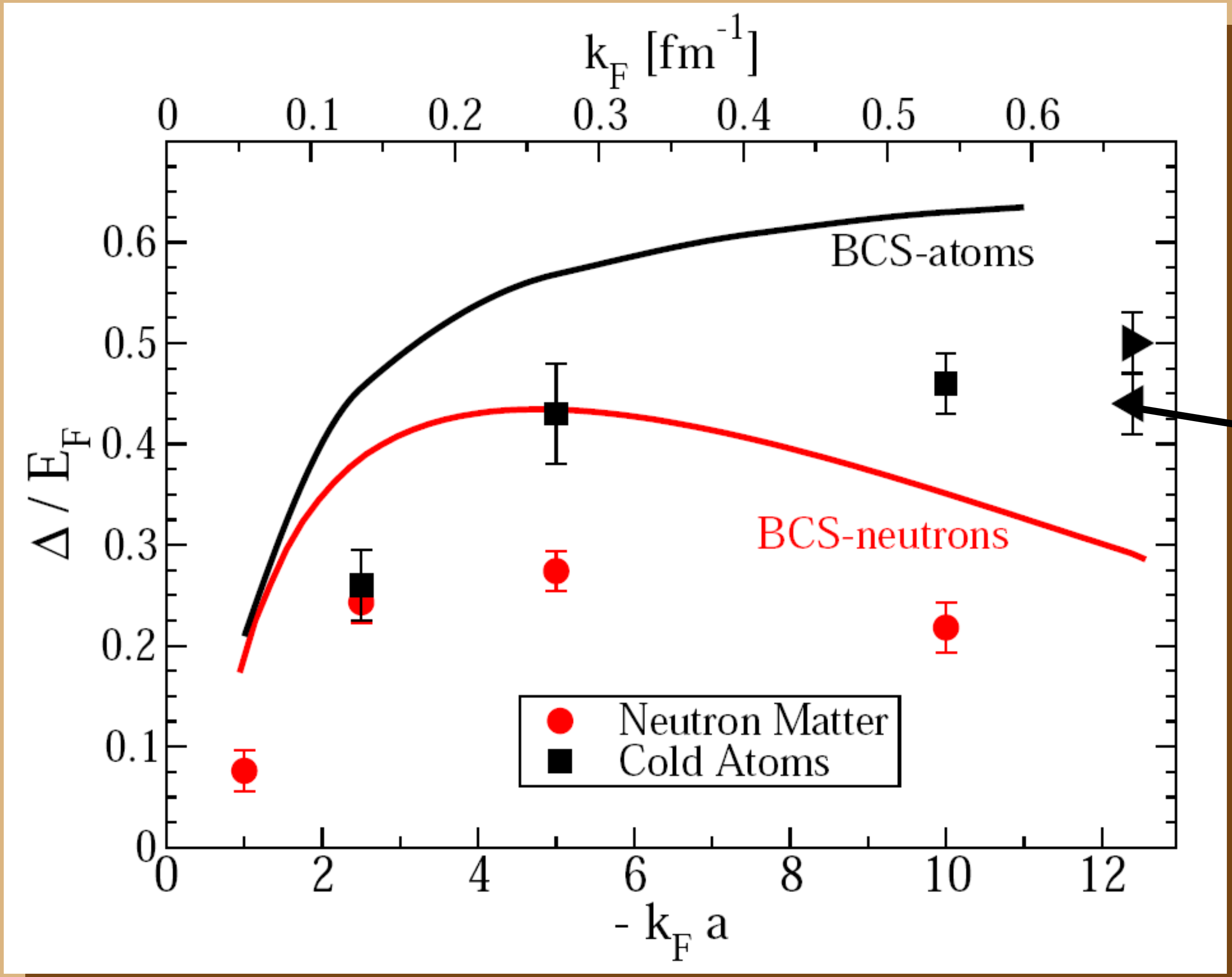
Connection:

Using “Feshbach” resonances one can tune the coupling

Credit: Thesis of Martin Zwierlein



Pairing gaps: results



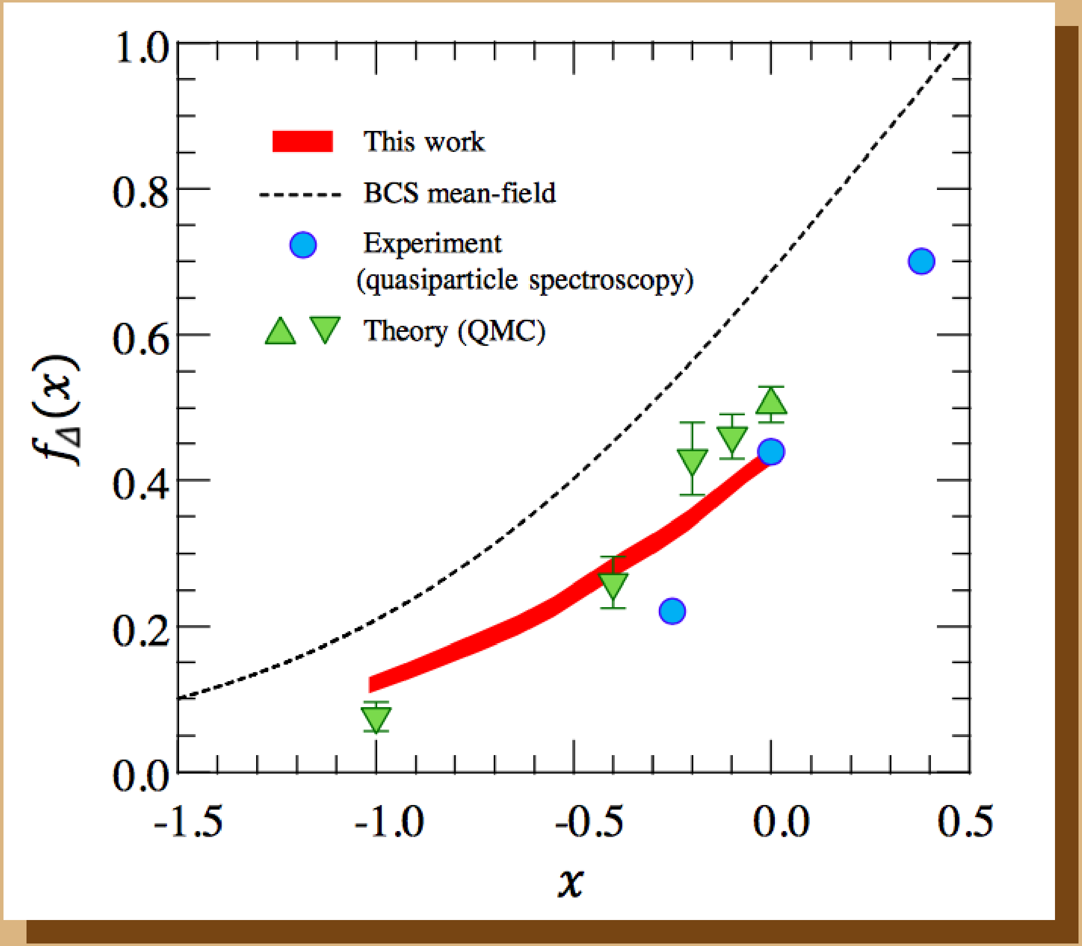
- Results identical at low density
- Range important at high density
- Two independent MIT experiments at unitarity

NEUTRONS

ATOMS

A. Gezerlis and J. Carlson, Phys. Rev. C **77**, 032801 (2008)
S. Gandolfi, A. Gezerlis, and J. Carlson, Ann. Rev. Nucl. Part. Sci. **65**, 303 (2015)

Experiment on cold-gas gaps away from unitarity



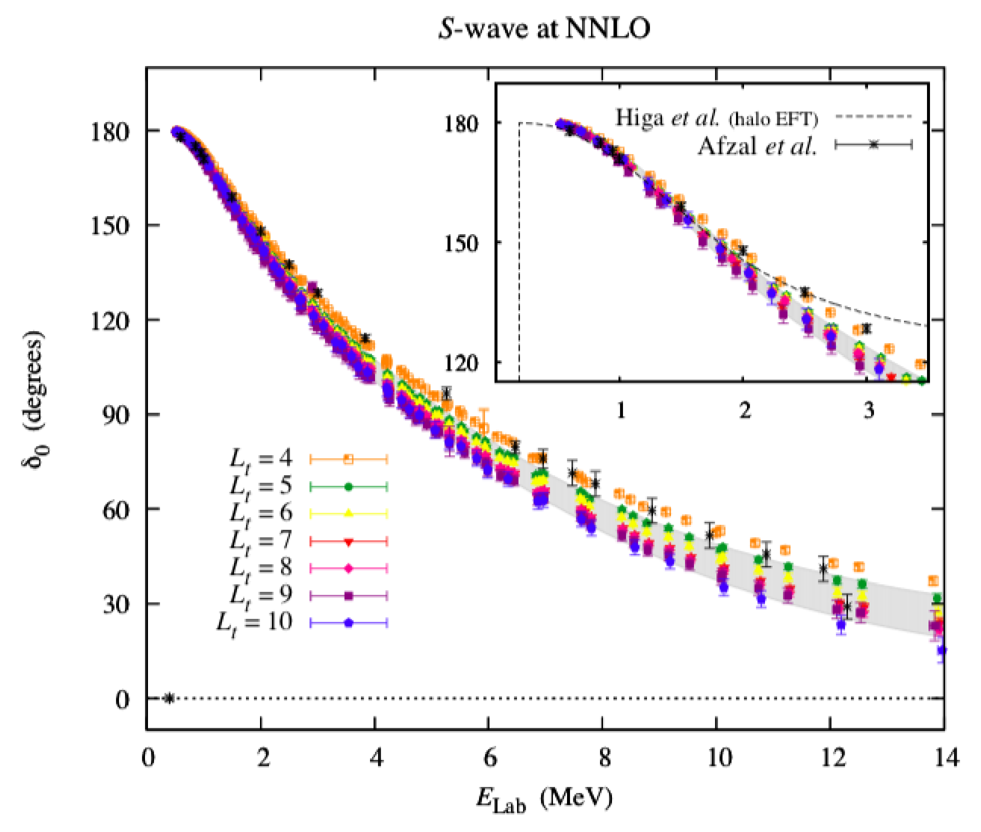
- New experiment at University of Tokyo
- ^{6}Li at $T/T_F < 0.06$
- Experimental extraction includes (some) beyond mean-field effects

ATOMS

M. Horikoshi et al, Phys. Rev. X **7**, 041004 (2017)

2. Alpha clustering in *ab initio* theories

Lattice EFT for α-α scattering



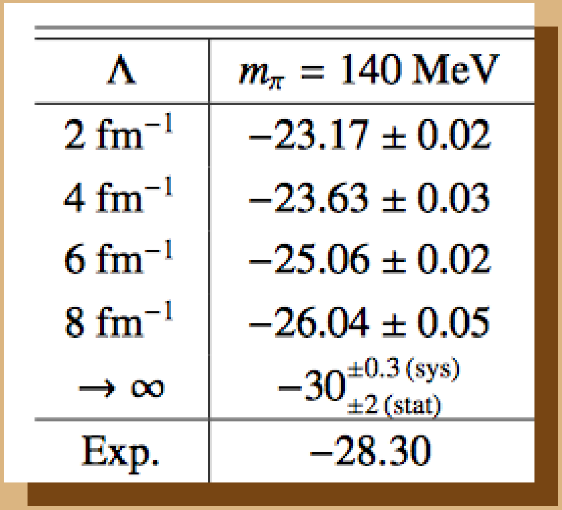
- NNLO chiral interaction
- 8Be ground state bound by a fraction of an MeV
- Inset shows Halo EFT with pointlike alpha particles

NUCLEONS

S. Elhatisari, D. Lee, G. Rupak, E. Epelbaum, H. Krebs, T. A. Lahde, T. Luu, U.-G.Meissner, Nature **528**, 111 (2015)

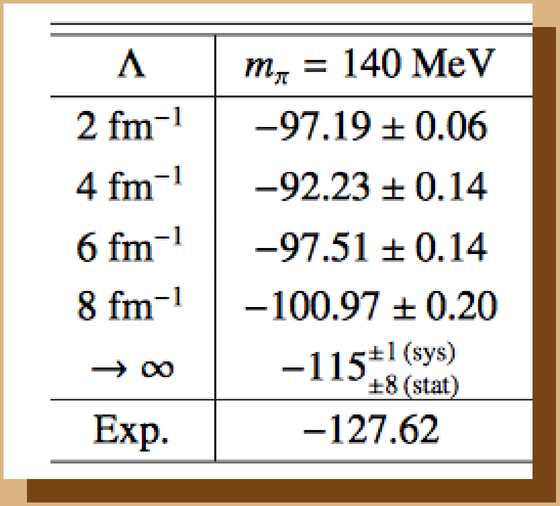
AFDMC with pionless EFT

4He



Λ	m_π = 140 MeV
2 fm^{-1}	-23.17 ± 0.02
4 fm^{-1}	-23.63 ± 0.03
6 fm^{-1}	-25.06 ± 0.02
8 fm^{-1}	-26.04 ± 0.05
$\to \infty$	$-30^{\pm 0.3\,\text{(sys)}}_{\pm 2\,\text{(stat)}}$
Exp.	-28.30

16O



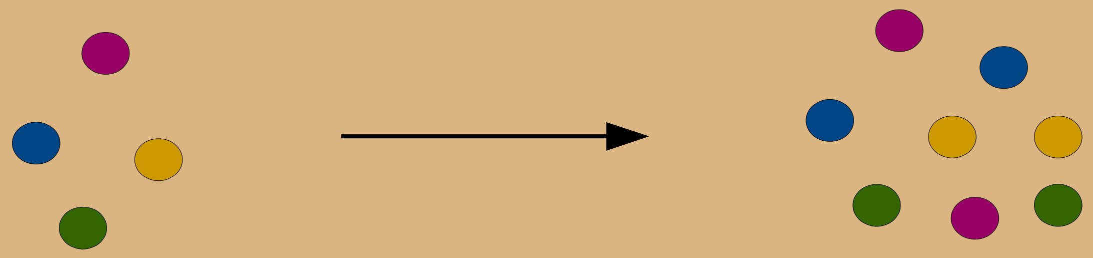
Λ	m_π = 140 MeV
2 fm^{-1}	-97.19 ± 0.06
4 fm^{-1}	-92.23 ± 0.14
6 fm^{-1}	-97.51 ± 0.14
8 fm^{-1}	-100.97 ± 0.20
$\to \infty$	$-115^{\pm 1\,\text{(sys)}}_{\pm 8\,\text{(stat)}}$
Exp.	-127.62

- AFDMC with simple wave function
- LO pionless EFT interaction (with 3NF)
- 16O tends to break up into 4He clusters

NUCLEONS

L. Contessi, A. Lovato, F. Pederiva, A. Roggero, J. Kirscher, U. van Kolck, Phys. Lett. **B 07**, 048 (2017)

QMC for 4 species



QMC for 4 species

Motivation

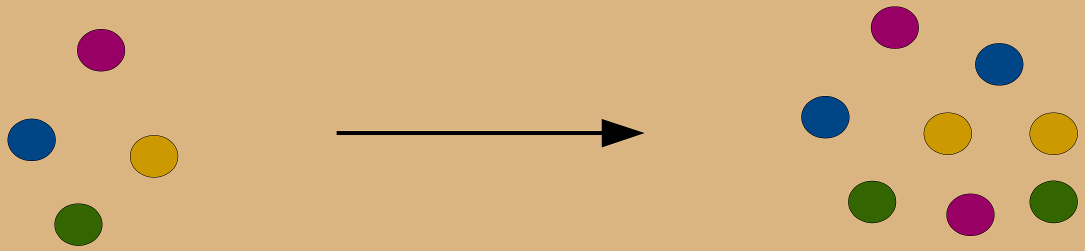
- Very successful cold Fermi atom experiments with few or many particles

- Nuclear physics around the unitary limit:
  S. Koenig, H. W. Griesshammer, H.-W. Hammer, U. van Kolck
  Phys. Rev. Lett. **118**, 202501 (2017)

- Unitary bosons from clusters to matter
  J. Carlson, S. Gandolfi, U. van Kolck, S. A. Vitiello
  Phys. Rev. Lett. **119**, 223002 (2017)

NUCLEONS

QMC for 4 species



Hamiltonian

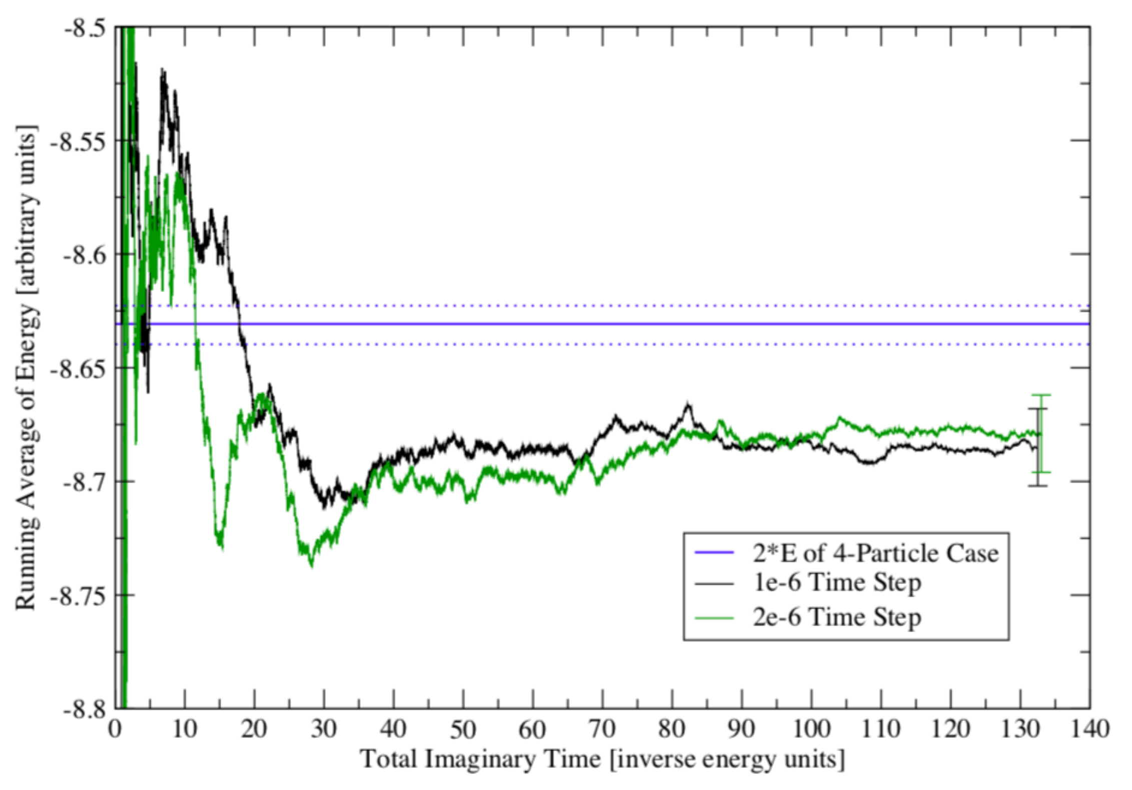
$$H = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk}$$

$$V_{ij} = V_2^0 \frac{\hbar^2}{m}\mu_2^2 \exp[-(\mu_2 r_{ij})^2/2]$$

$$V_{ijk} = V_3^0 \frac{\hbar^2}{m}\left(\frac{\mu_3}{2}\right)^2 \exp[-(\mu_3 R_{ijk}/2)^2/2]$$

N. B. Fermions are not bosons [sic]

QMC for SU(4): 8 particles



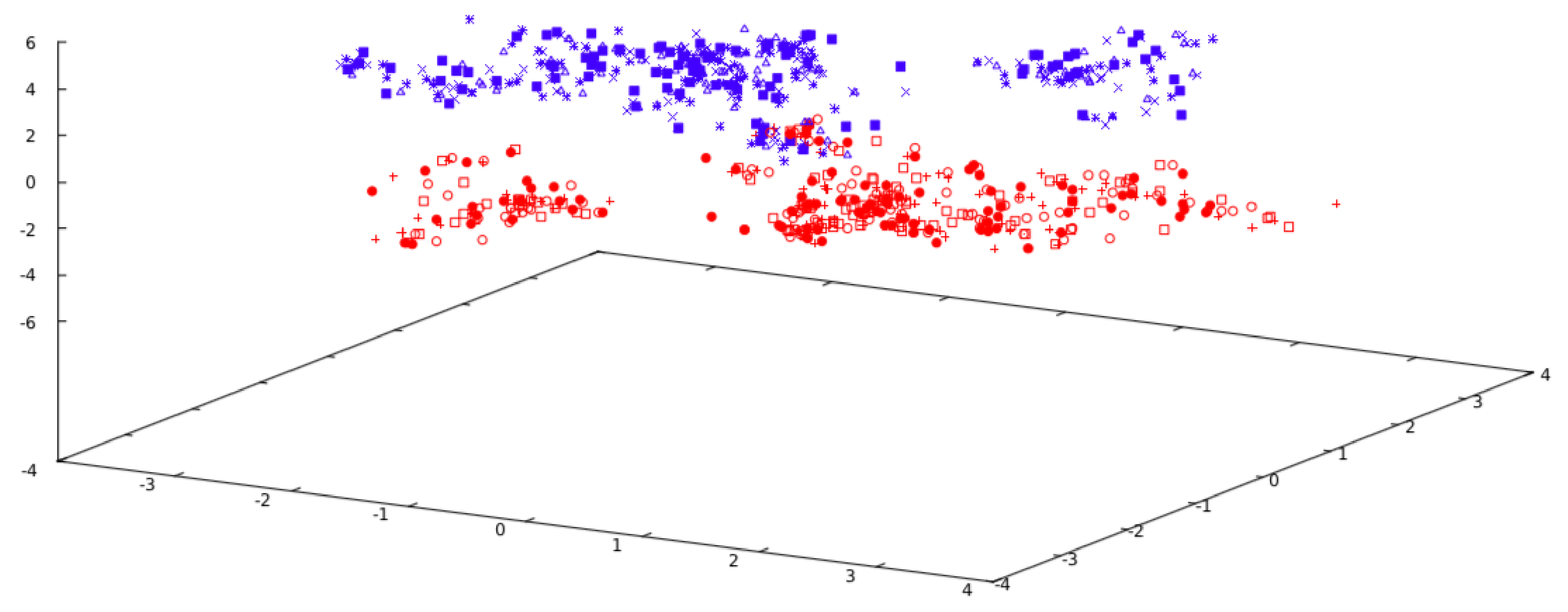
- Pionless EFT with NN+NNN
- Careful time-step extrapolation
- 8Be found to be (barely) bound wrt to α decay, already at LO

W. Dawkins, J. Carlson, U. van Kolck, A. Gezerlis, *in preparation* (2019)

NUCLEONS

QMC for SU(4): 8 particles

The two clusters are interpenetrating



NUCLEONS

W. Dawkins, J. Carlson, U. van Kolck, A. Gezerlis, *in preparation* (2019)

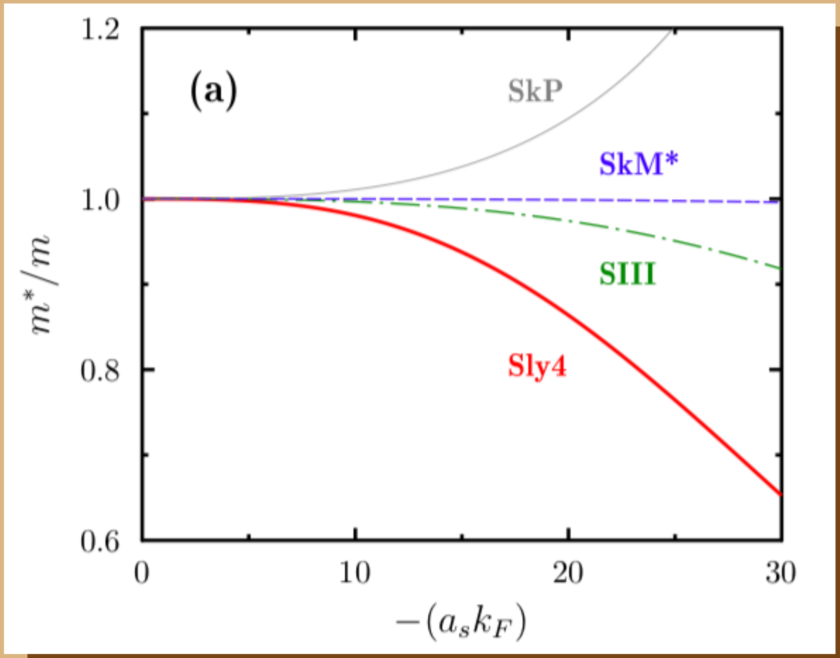
3. Effective mass extraction

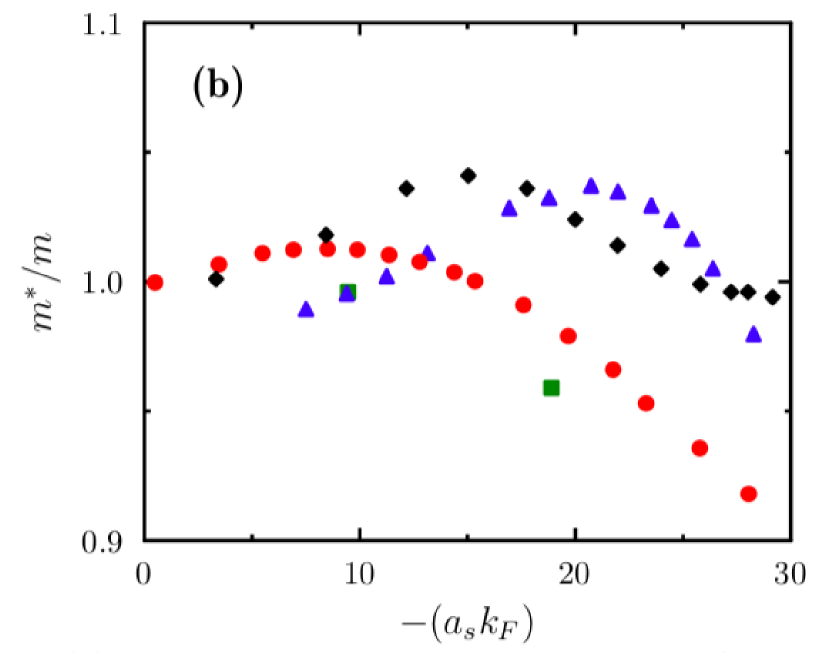
Neutron matter effective mass

Motivation

$$\frac{m^*}{m} = \frac{m^*_E}{m} \cdot \frac{m^*_k}{m}$$

- Many definitions and many applications, see:
  B.-A. Li, B. J. Cai, L.-W. Chen, J. Xu, Prog. Part. Nucl. Phys. 99, 29 (2018)
- Many extractions, both in Skyrme EDF and using *ab initio*, see
  A. Boulet and D. Lacroix, Phys. Rev. C 97, 014301 (2018)



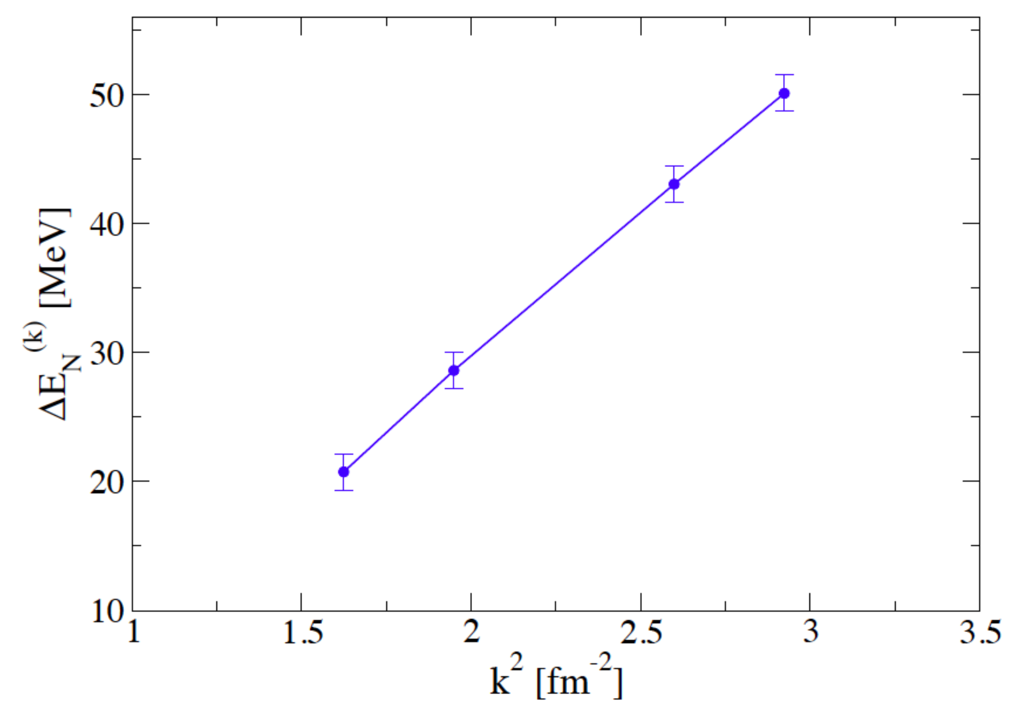


Neutron matter quasiparticle dispersion

Definition

$$\Delta T_N^{(k)} \equiv T_{N+1}^{(k)} - T_N + \frac{2}{5} E_F$$

$$\Delta E_N^{(k)} \equiv E_{N+1}^{(k)} - E_N + \frac{2}{5} \xi E_F$$



AFDMC calculation

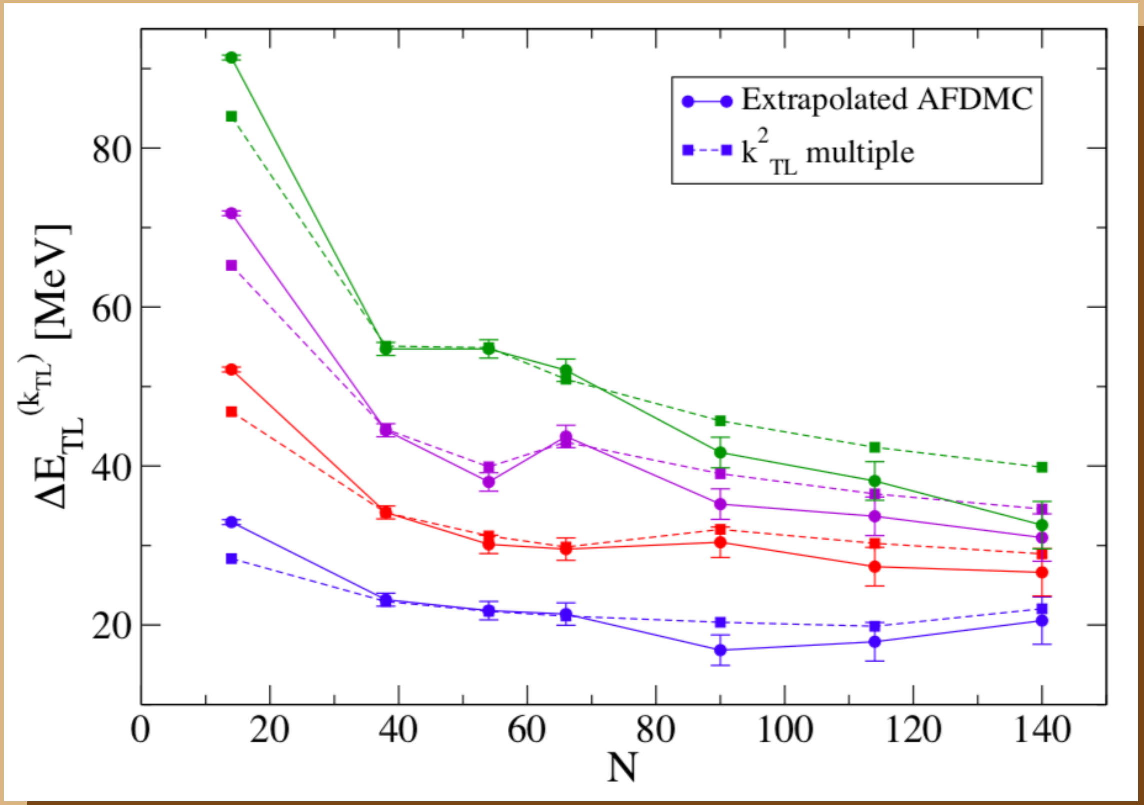
NEUTRONS

M. Buraczynski, N. Ismail, and A. Gezerlis, Phys. Rev. Lett. **122**, 152701 (2019)

Neutron matter quasiparticle dispersion

Transition to the Thermodynamic Limit (TL) understood reasonably well

$$\Delta E_{TL}^{(k_{TL})} = \Delta E_{N}^{(k)} - \Delta T_{N}^{(k)} + \frac{\hbar^2 k_{TL}^2}{2m}$$



AFDMC calculation

NEUTRONS

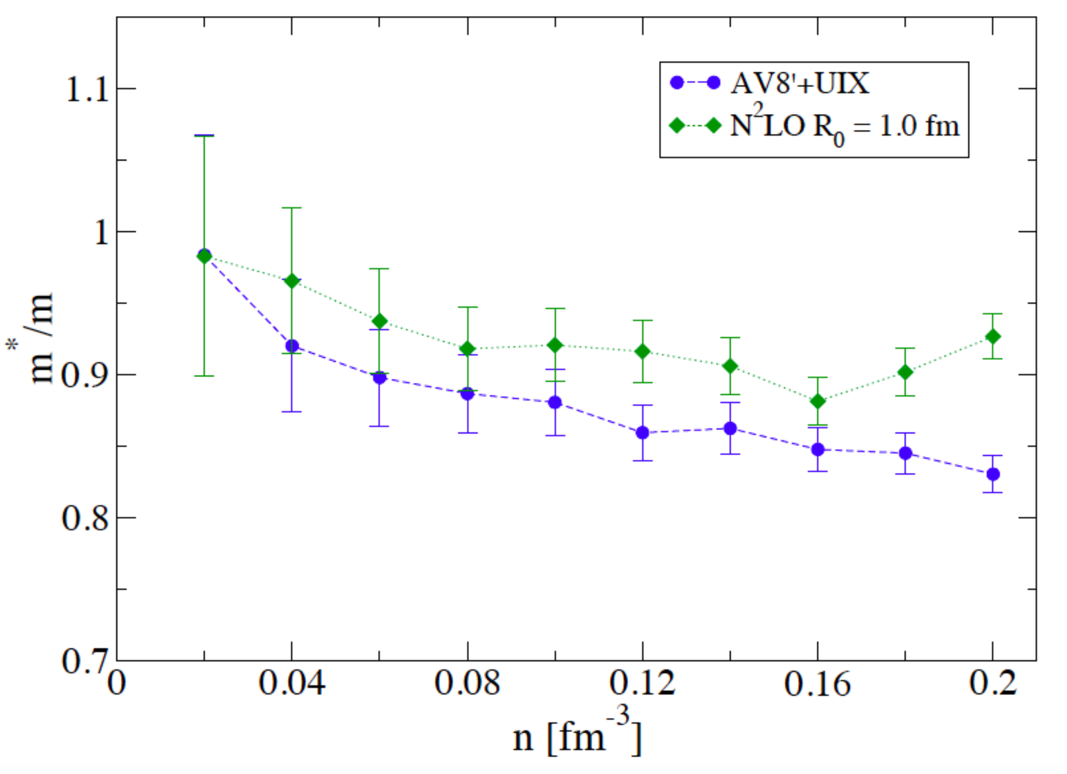
M. Buraczynski, N. Ismail, and A. Gezerlis, Phys. Rev. Lett. **122**, 152701 (2019)

Neutron matter effective mass

Extraction from AFDMC

$$\Delta T_N^{(k)} \equiv T_{N+1}^{(k)} - T_N + \frac{2}{5}E_F = \frac{\hbar^2 k^2}{2m}$$

$$\Delta E_N^{(k)} \equiv E_{N+1}^{(k)} - E_N + \frac{2}{5}\xi E_F = \frac{\hbar^2 k^2}{2m^*}$$



- Error bar tries to reflect both systematics and fit to the quadratic
- Many other potentials also used (not shown)

NEUTRONS

M. Buraczynski, N. Ismail, and A. Gezerlis, Phys. Rev. Lett. **122**, 152701 (2019)

Conclusions

- Rich connections between physics of nuclei and that of compact stars
- Exciting time in terms of interplay between nuclear interactions, QCD, and many-body approaches
- Ab initio and phenomenology are mutually beneficial

Acknowledgments

Collaborators

Guelph

- Mateusz Buraczynski
- Will Dawkins
- Nawar Ismail

IPN Orsay

- Denis Lacroix
- Bira van Kolck

Darmstadt

- Joel Lynn
- Achim Schwenk

LANL

- Joe Carlson
- Stefano Gandolfi
- Ingo Tews

Acknowledgments

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

- Mateusz Buraczynski
- Will Dawkins
- Nawar Ismail

IPN Orsay

- Denis Lacroix
- Bira van Kolck

Darmstadt

- Joel Lynn
- Achim Schwenk

LANL

- Joe Carlson
- Stefano Gandolfi
- Ingo Tews