Simplified microscopic and effective interactions in Quantum Monte Carlo

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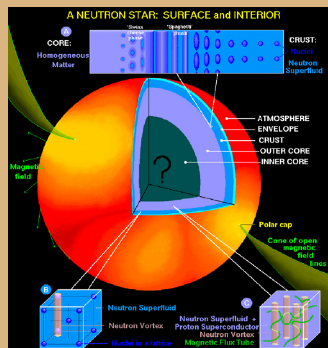
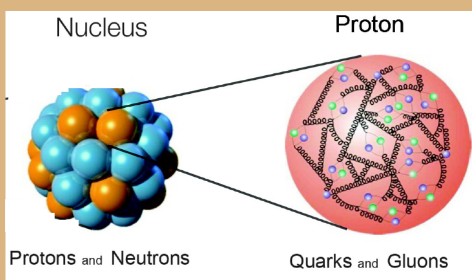
"Progress in Ab Initio Techniques in Nuclear Physics" workshop
TRIUMF, Vancouver, BC
February 26, 2019

Outline

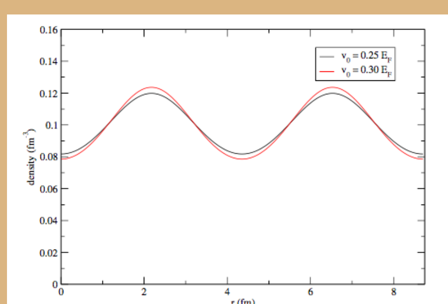


Credit: Dany Page

Motivation

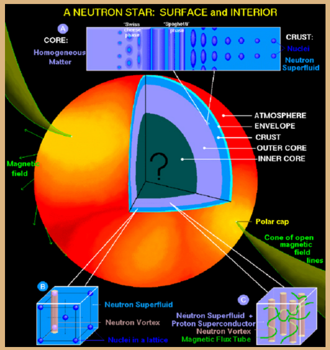


Nuclear methods



Recent results

Outline



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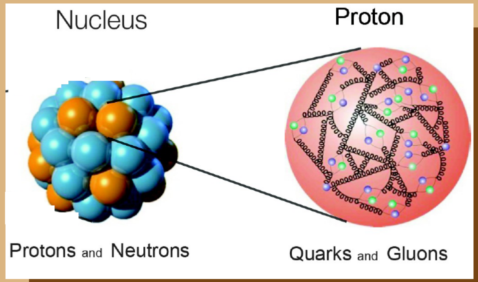
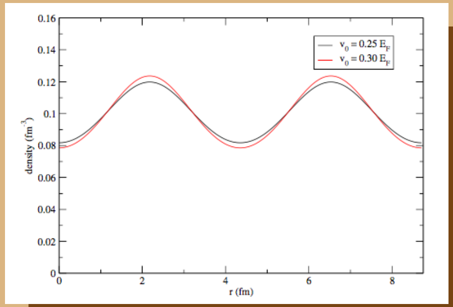
Motivation



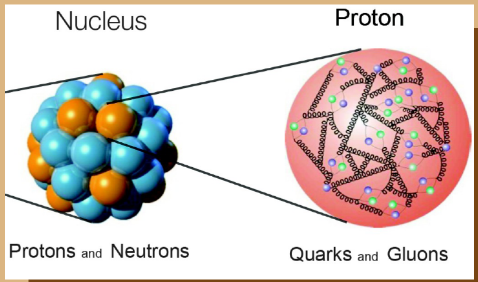
Nuclear methods



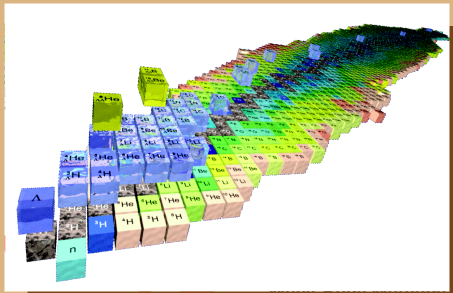
Recent results

Physical systems studied

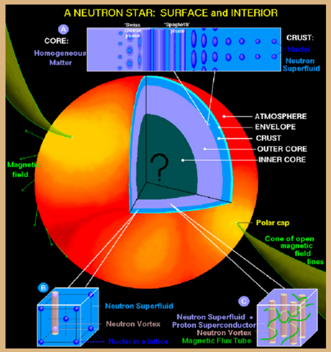
Nuclear forces



Nuclear structure

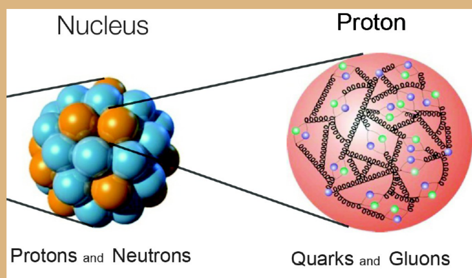


Nuclear astrophysics

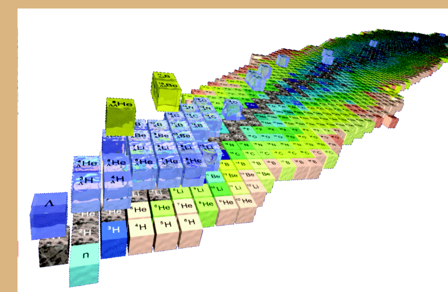


Physical systems studied

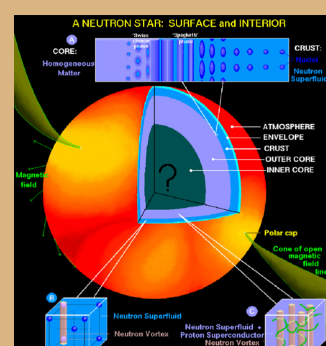
Nuclear forces

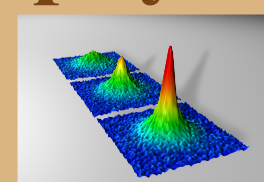


Nuclear structure



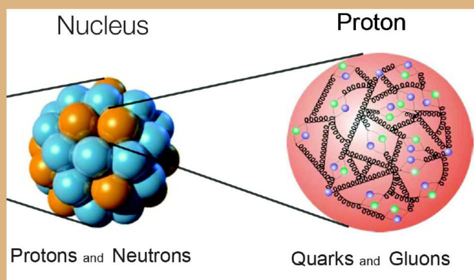
Nuclear astrophysics



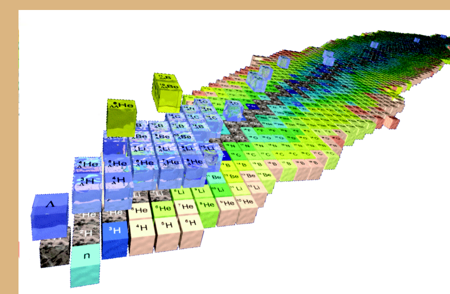


Physical systems studied

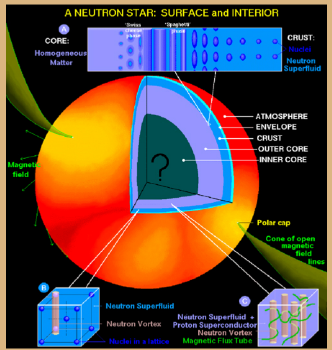
Few nucleons

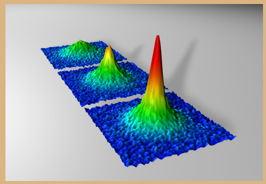


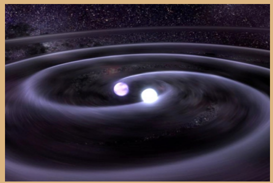
Many nucleons



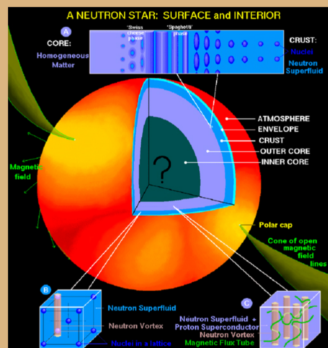
Very many nucleons





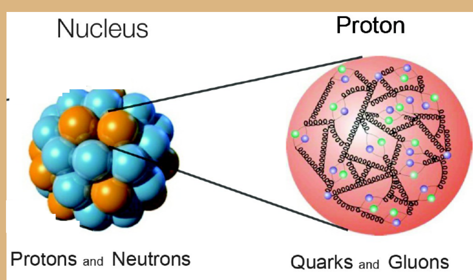


Outline

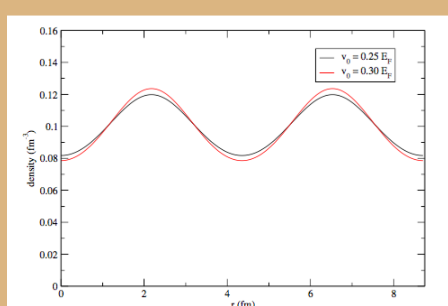


Credit: Dany Page

Motivation



Nuclear methods



Recent results

Nuclear interactions 1

Historically

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

Phenomenological

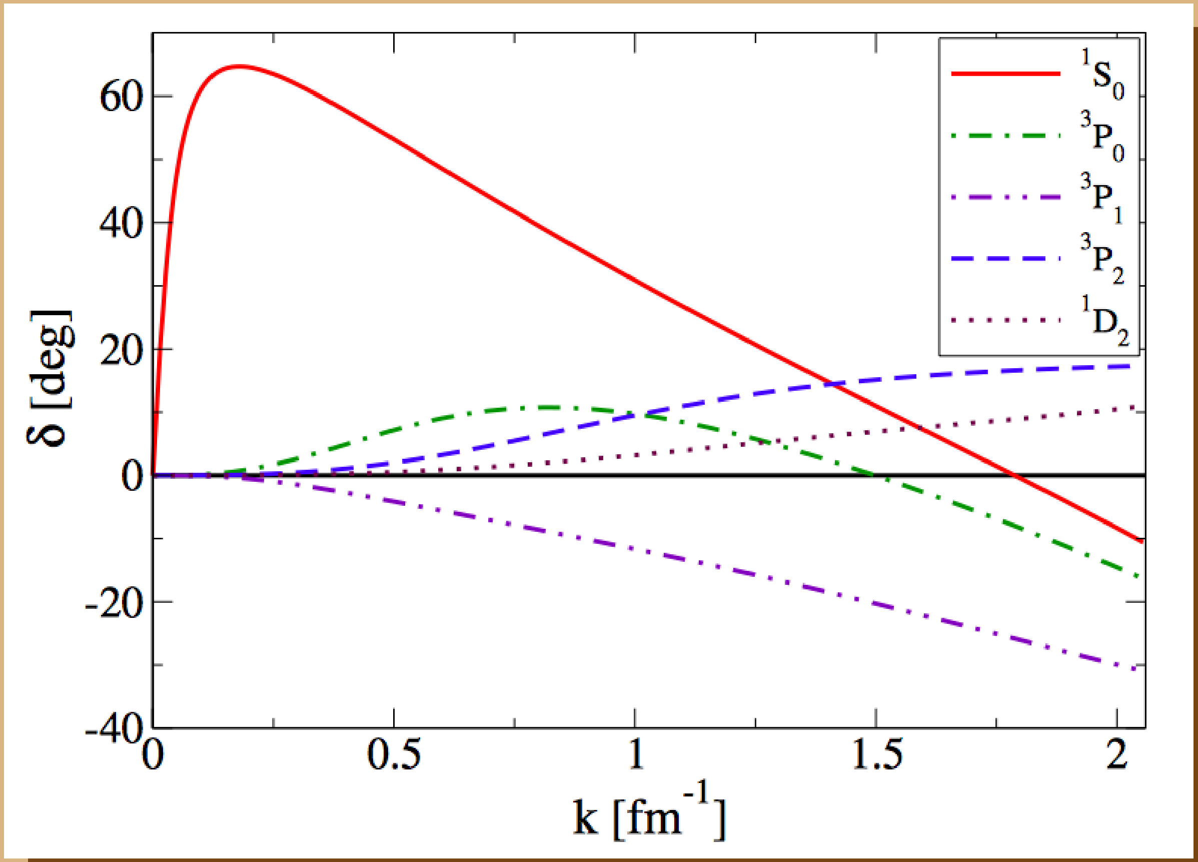
NN interaction fit to N-body experiment

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

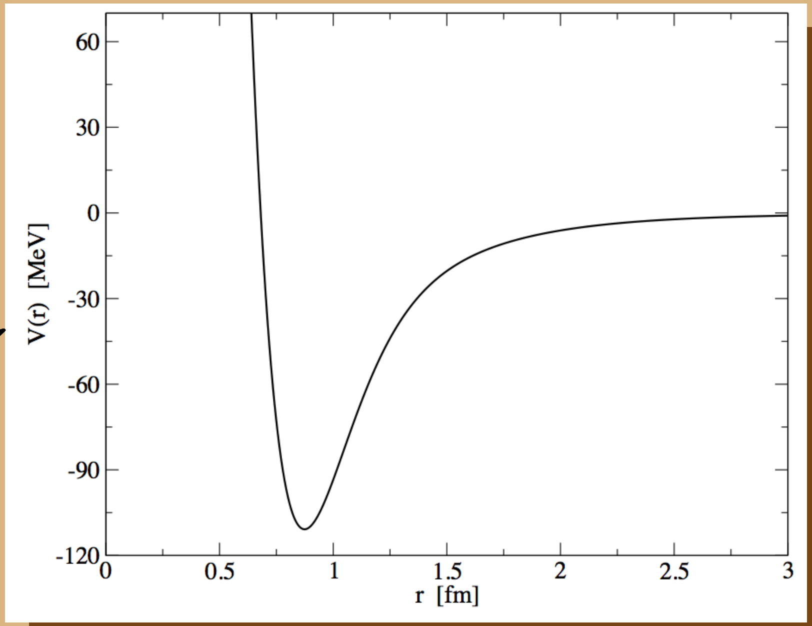
Nuclear interactions 2

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

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

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

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



How to go beyond?

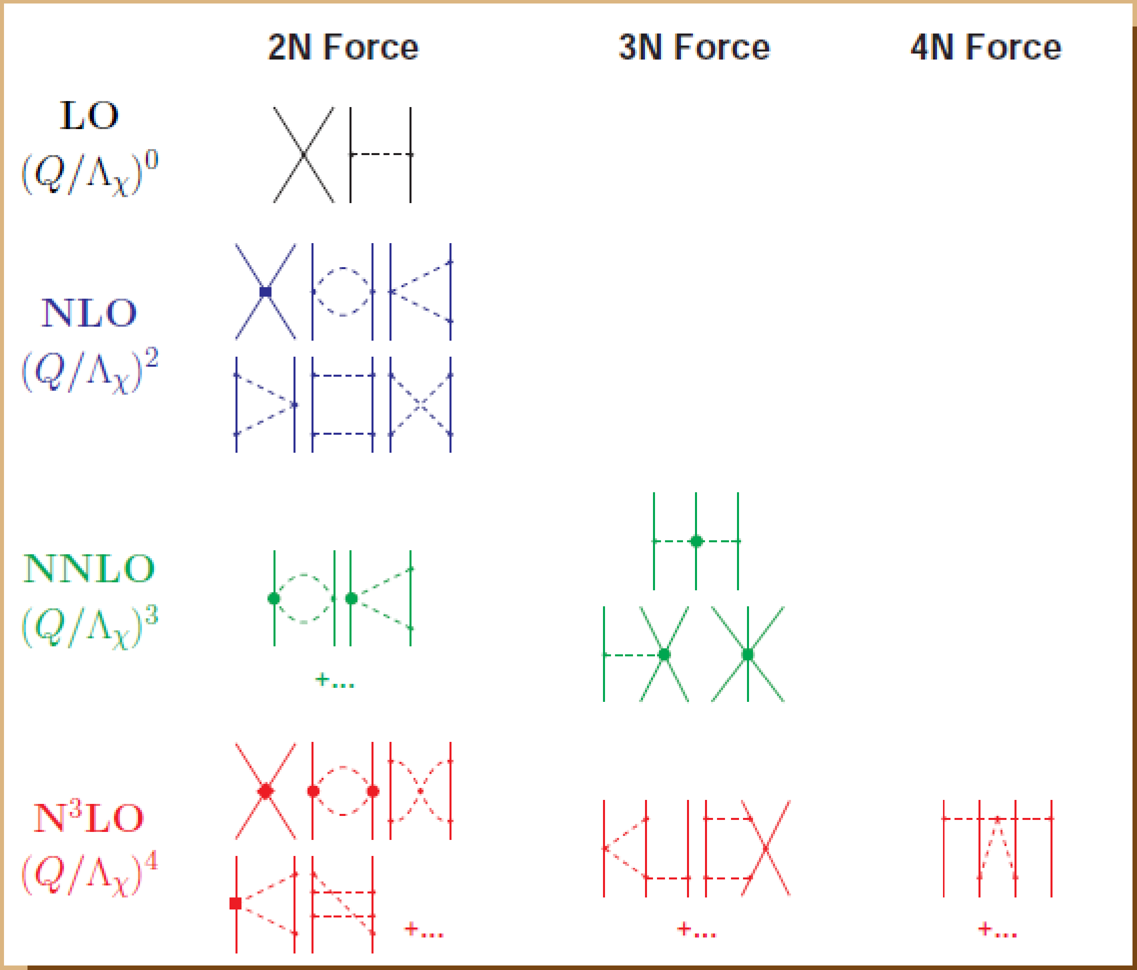
Historically, fit NN interaction to N-body experiment

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

Effective field theory

Nuclear interactions 3



- 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 still an open question

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

Main many-body methods employed (by me)

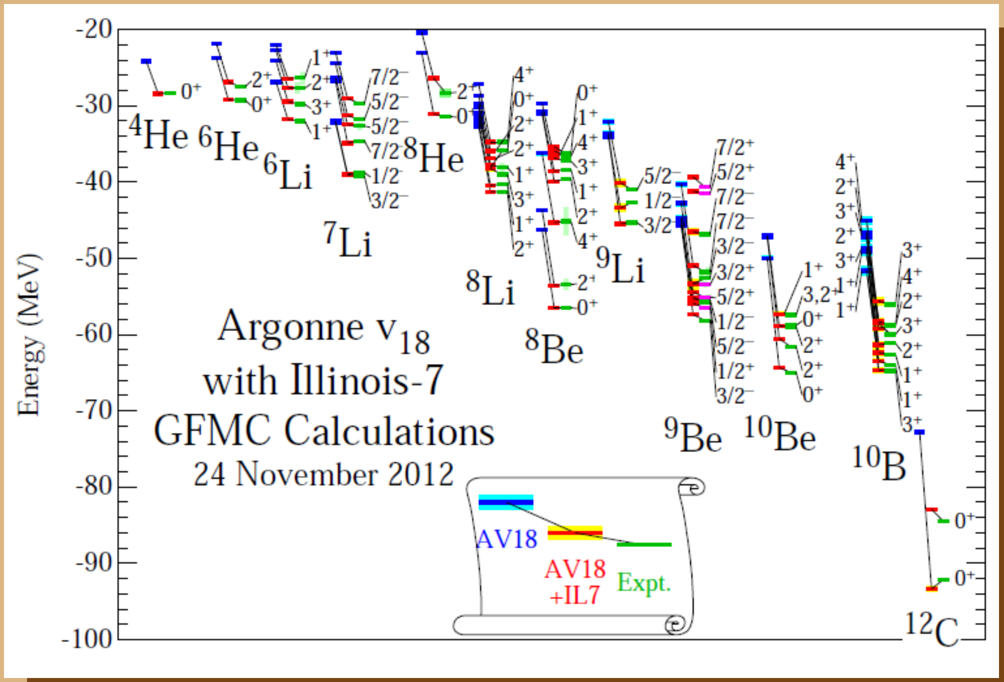
Two complementary methods

Quantum Monte Carlo

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

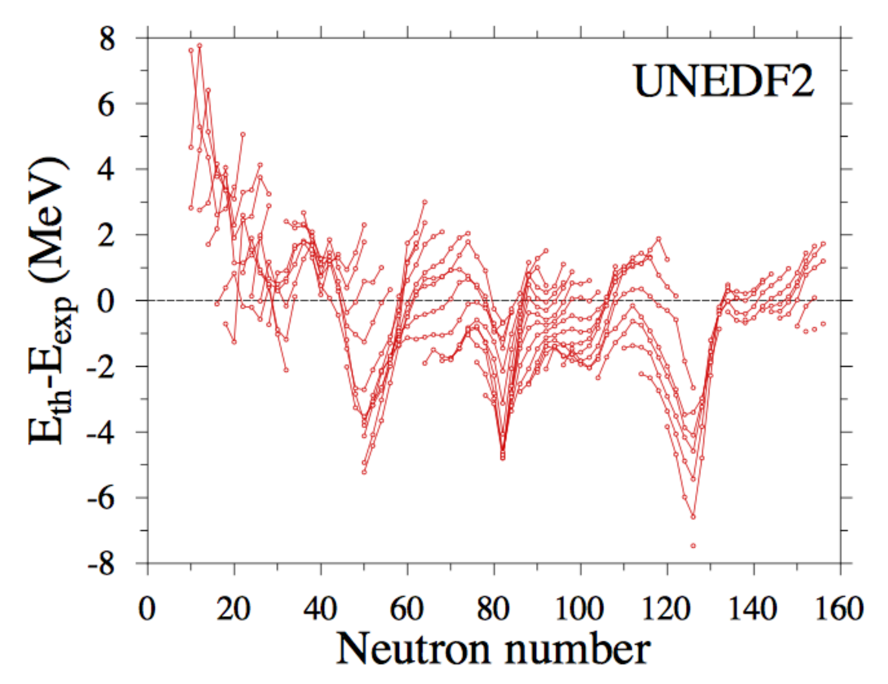
$$\Psi(\tau \to \infty) = \lim_{\tau \to \infty} e^{-(\mathcal{H}-E_T)\tau} \Psi_V$$

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



Credit: Steve Pieper

Two complementary methods



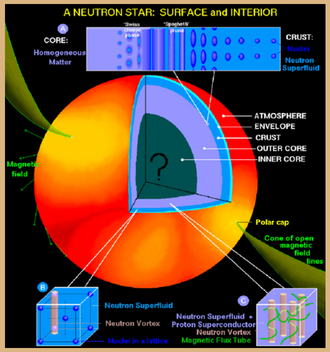
Credit: W. Nazarewicz

Density Functional Theory

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

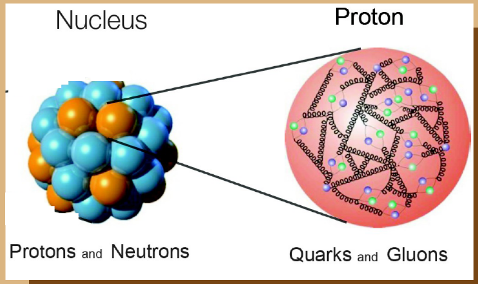
$$E = \int d^3r \, \{\mathcal{E}[\rho(\mathbf{r})] + \rho(\mathbf{r})V_{\text{ext}}(\mathbf{r})\}$$

Outline

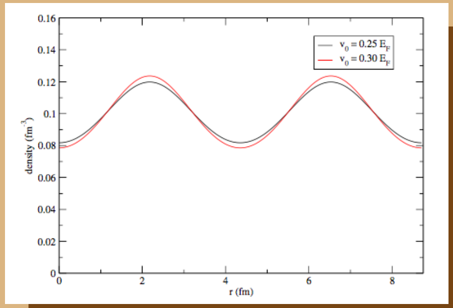


Credit: Dany Page

Motivation



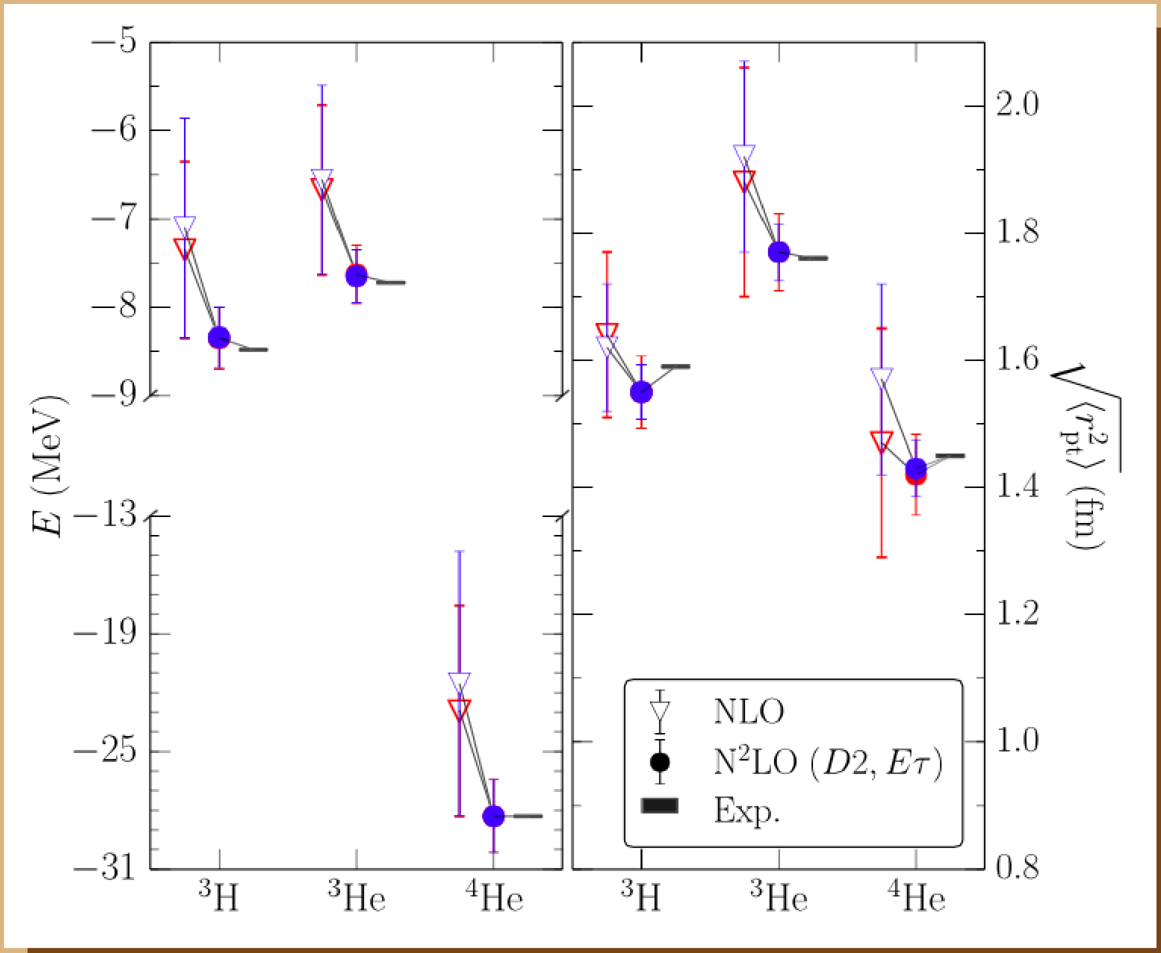
Nuclear background



Recent results

1. QMC with chiral or pionless EFT for nuclei

Nuclear GFMC with chEFT: NN+3NF



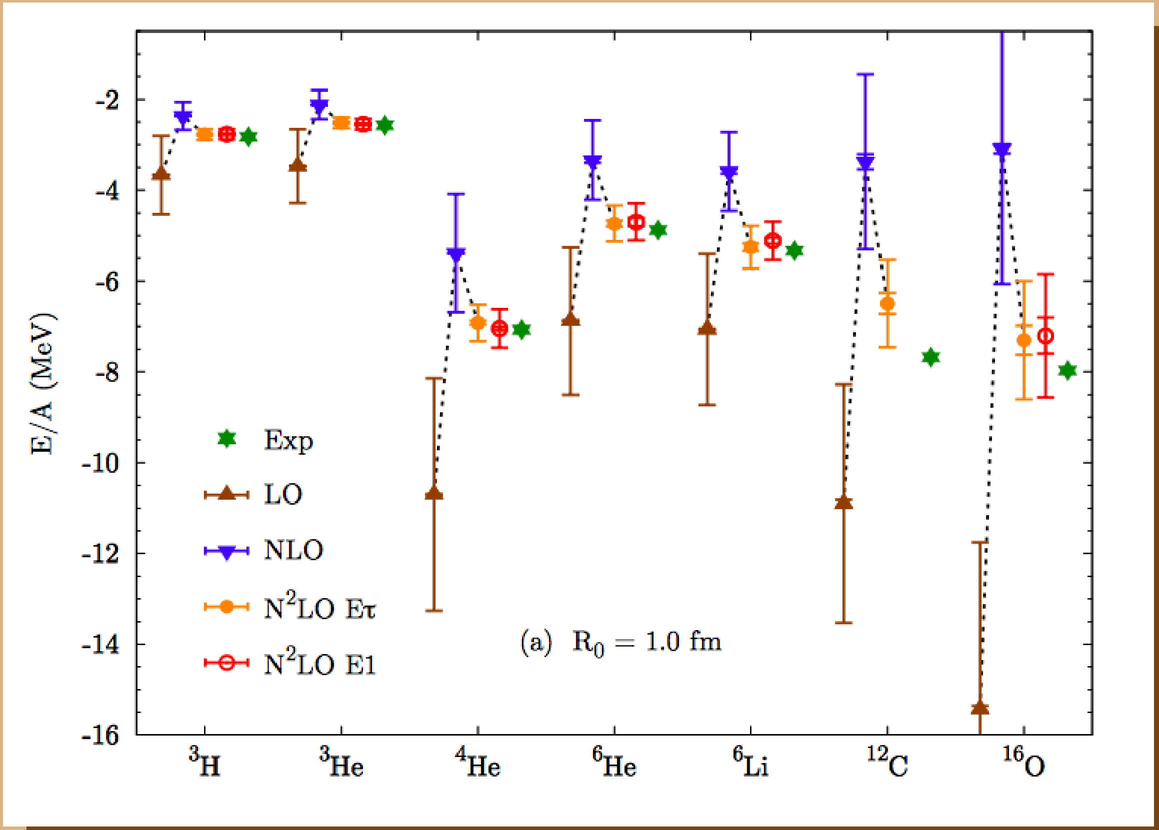
- Use c_D and c_E we fit
- Shown are both binding energies and point proton radii
- Things look reasonably good

NUCLEONS

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

J. E. Lynn, I. Tews, J. Carlson, S. Gandolfi, A. Gezerlis, K. E. Schmidt, A. Schwenk, I. Tews, Phys. Rev. C **96**, 054007 (2017)

AFDMC with chEFT: NN+3NF

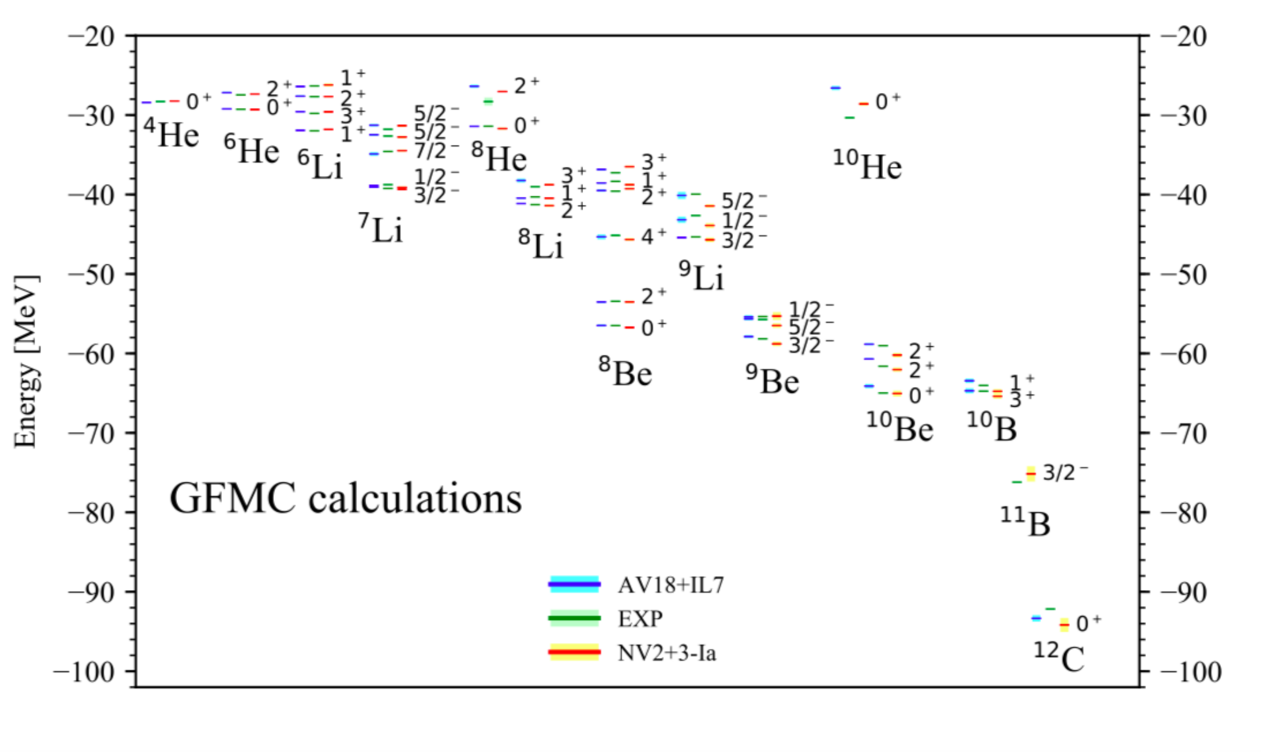


- AFDMC with better wave function
- Same local chiral EFT interactions as above
- Can be pushed to heavier masses

NUCLEONS

D. Lonardoni et al, Phys. Rev. C **97**, 044318 (2018)

Nuclear GFMC with chEFT

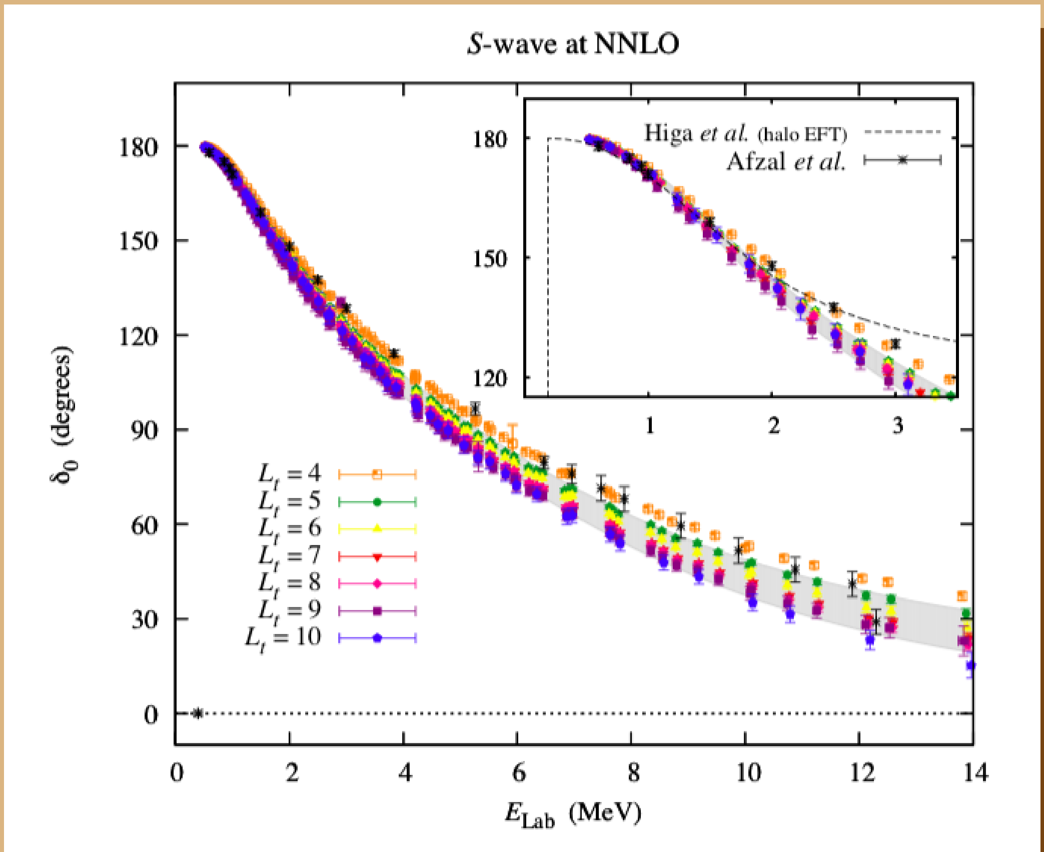


- GFMC with very good wave functions
- Different local chiral EFT interactions than above
- 37 states shown, with 60 more probed

NUCLEONS

M. Piarulli et al, Phys. Rev. Lett. **120**, 052503 (2018)

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
→ ∞	$-30^{\pm 0.3\,(sys)}_{\pm 2\,(stat)}$
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
→ ∞	$-115^{\pm 1\,(sys)}_{\pm 8\,(stat)}$
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)

Coupled Cluster pionless EFT

NLO $NN + NNN$							
$\hbar\omega$	Λ	$E(^3\text{H})$	$r(^3\text{H})$	$E(^3\text{He})$	$r(^3\text{He})$	$E(^4\text{He})$	$r(^4\text{He})$
5	306.52	53.9	1.55	53.1	1.55	99.0	1.55
10	433.48	53.9	1.14	52.9	1.16	89.9	1.17
22	642.96	53.9	1.04	52.7	1.13	89.7	1.34
40	866.97	53.9	1.17	53.1	1.29	109.7	1.33

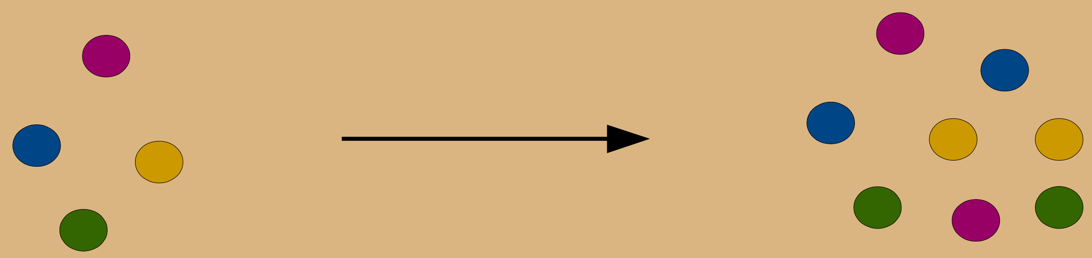
		^{16}O		^{40}Ca	
$\hbar\omega$	Λ	$N_1, N_3 = 12$	$N_1, N_3 = 14$	$N_1, N_3 = 12$	$N_1, N_3 = 14$
5	232.35	174.1	174.8	562.5	569.2
10	328.59	136.8	136.2	421.8	415*
22	487.38	143.1	143.1	405.8	405.8
40	657.19	144.7	146.2	372.2	400.0

- For 4He, CCSD in agreement with NCSM
- At LO, 16O and 40Ca not bound wrt decay into α's
- Oscillator spacings of 10 MeV and up most dependable

NUCLEONS

A. Bansal, S. Binder, A. Ekstrom, G. Hagen, G. R. Jansen, T. Papenbrock, Phys. Rev. C **98**, 054301 (2018)

QMC for 4 species



QMC for 4 species

Motivation

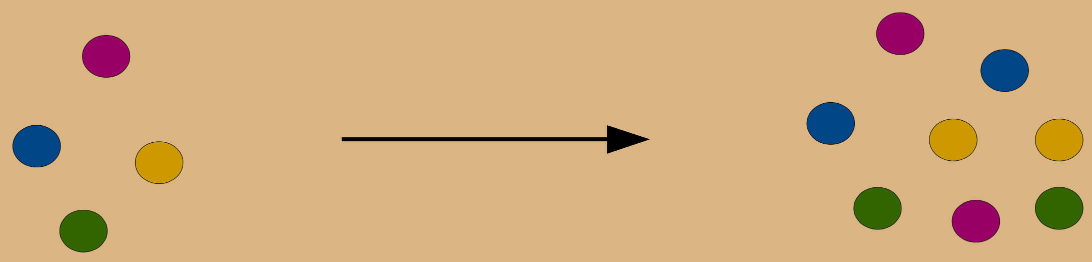
- Very successful cold Fermi atom experiments with few or many particles

- 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



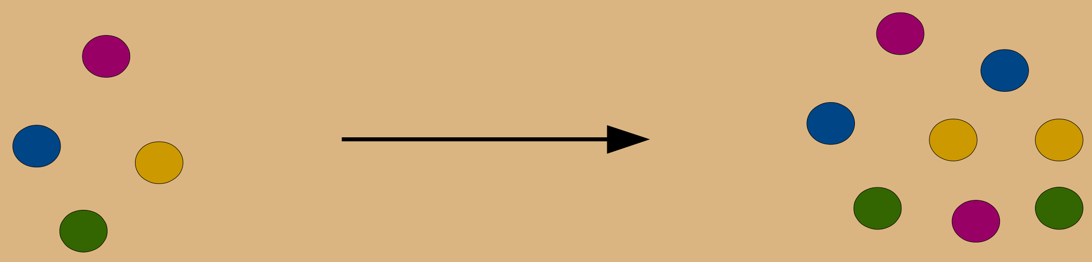
Hamiltonian

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

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

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

QMC for 4 species



Hamiltonian

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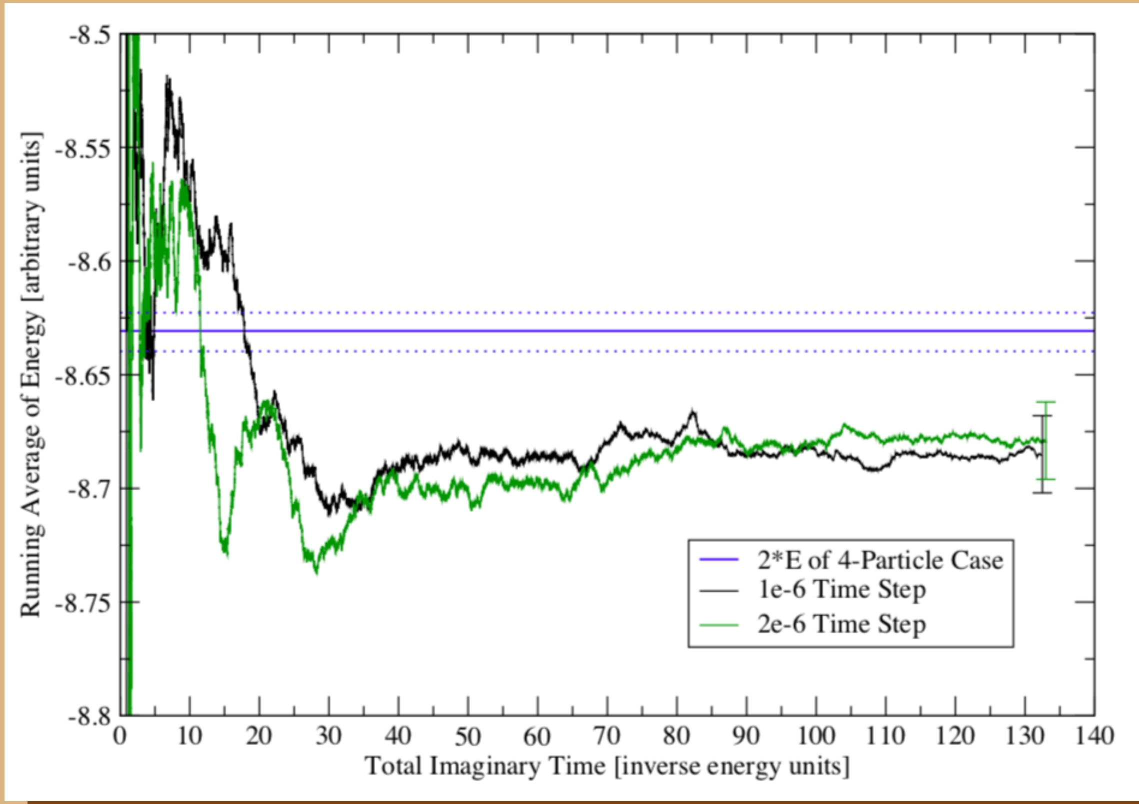
$$V_{ij} = V_2^0 \frac{\hbar^2}{m}\mu_2^2 \exp[-(\mu_2 r_{ij})^2/2]$$

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

N. B. Fermions are not bosons [sic]

QMC for SU(4): 8 particles



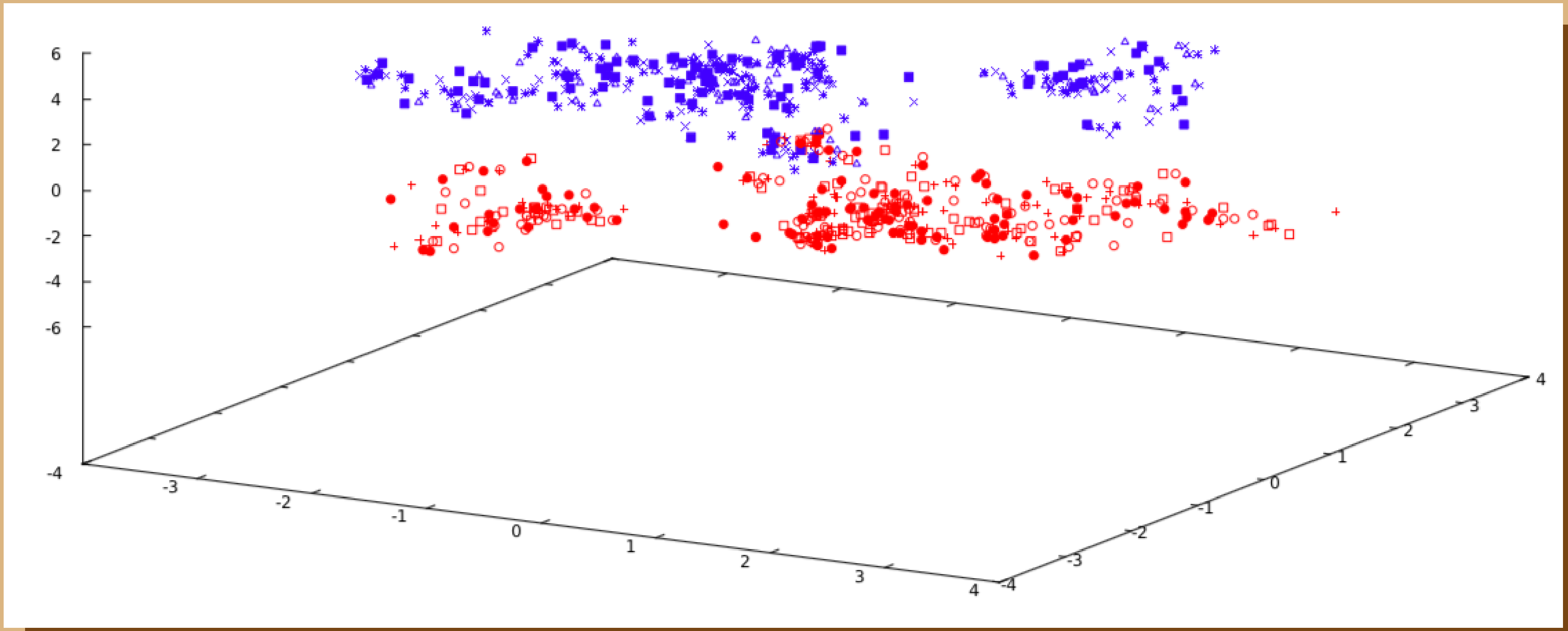
- Pionless EFT with NN+NNN
- Careful time-step extrapolation
- 8Be found to be (barely) bound wrt to α decay, already at LO

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

NUCLEONS

QMC for SU(4): 8 particles

The two clusters are interpenetrating



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

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2. Effective mass in neutron matter

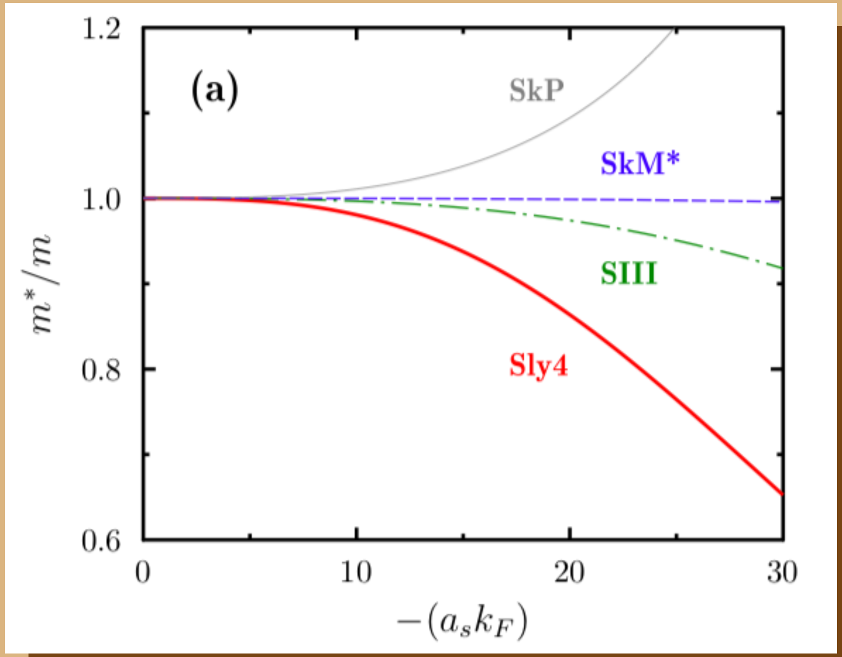
Neutron matter effective mass

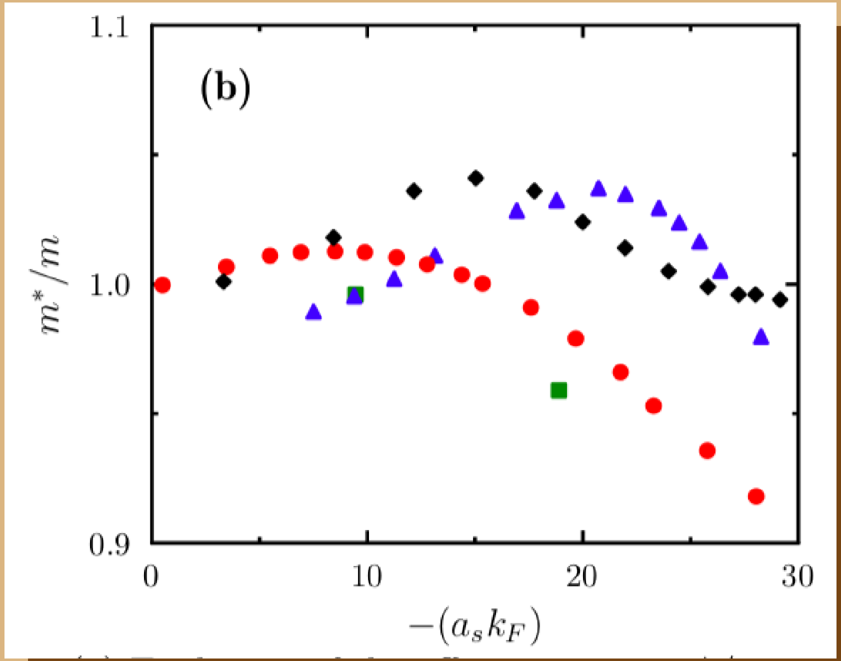
Motivation

$$\frac{m^*}{m} = \frac{m_E^*}{m} \cdot \frac{m_k^*}{m}$$

- 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)



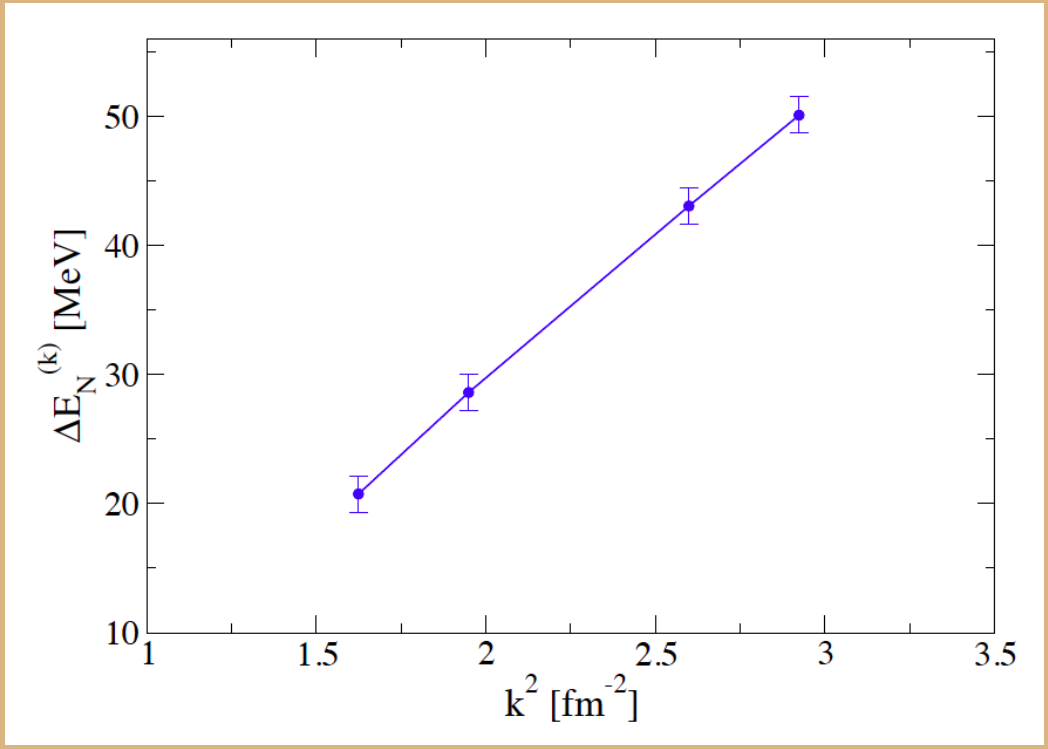


Neutron matter quasiparticle dispersion

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

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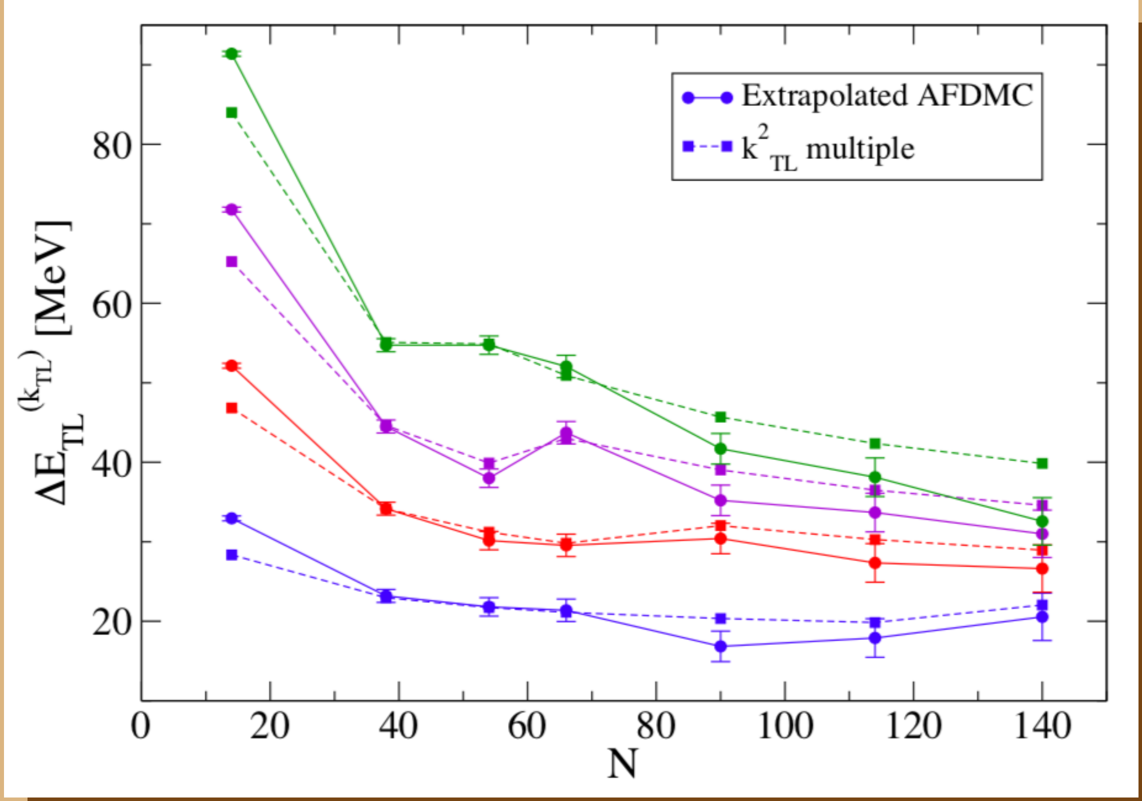
M. Buraczynski, N. Ismail, and A. Gezerlis, *submitted to* Phys. Rev. Lett.
arXiv:1901.00870

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

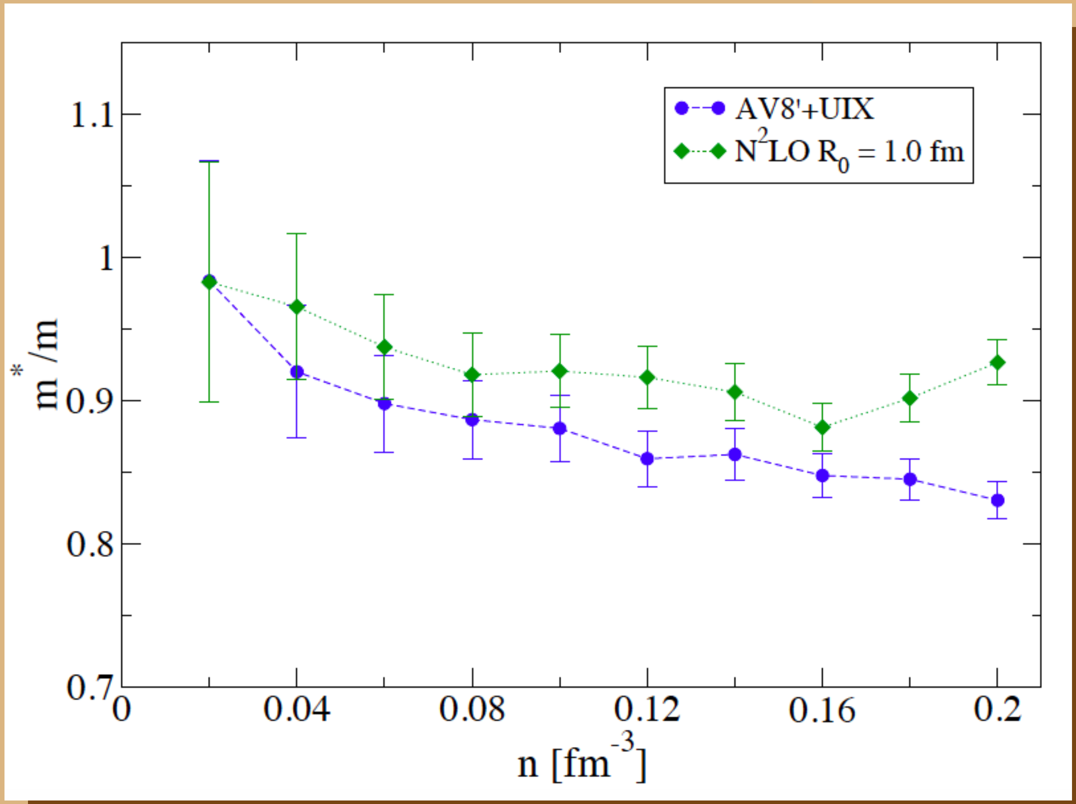
M. Buraczynski, N. Ismail, and A. Gezerlis, *submitted to* Phys. Rev. Lett. arXiv:1901.00870

Neutron matter effective mass

Extraction from AFDMC

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

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



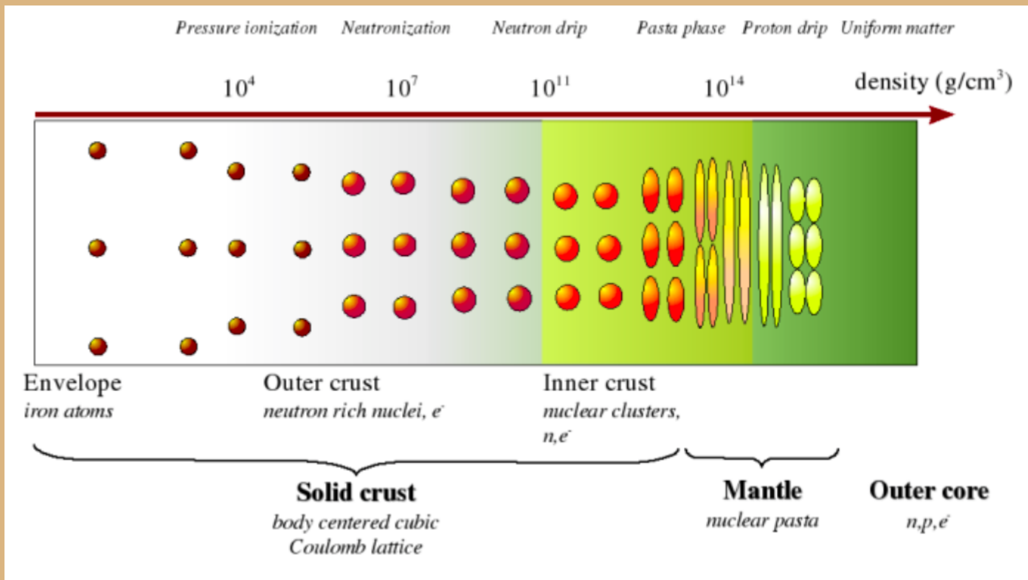
- Error bar tries to reflect both systematics and fit to the quadratic
- Many other potentials also used (not shown)

NEUTRONS

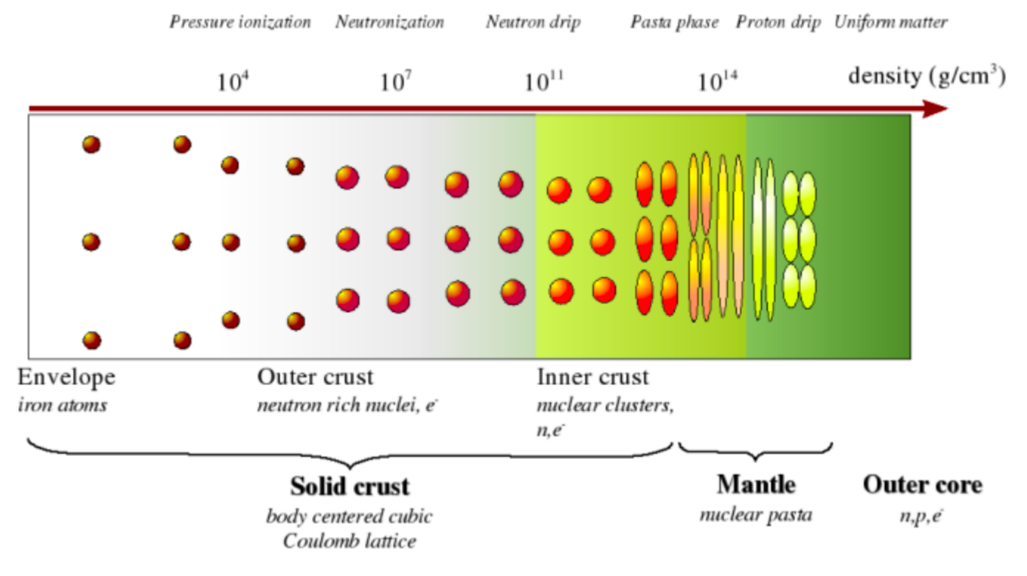
M. Buraczynski, N. Ismail, and A. Gezerlis, *submitted to* Phys. Rev. Lett. arXiv:1901.00870

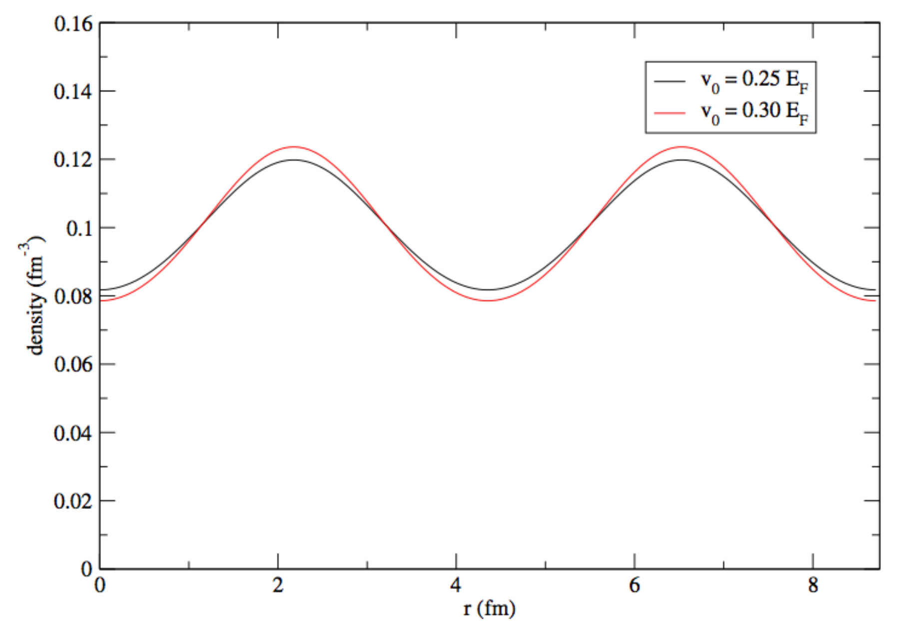
3. Static response of neutron matter

Neutron star crusts inhomogeneous

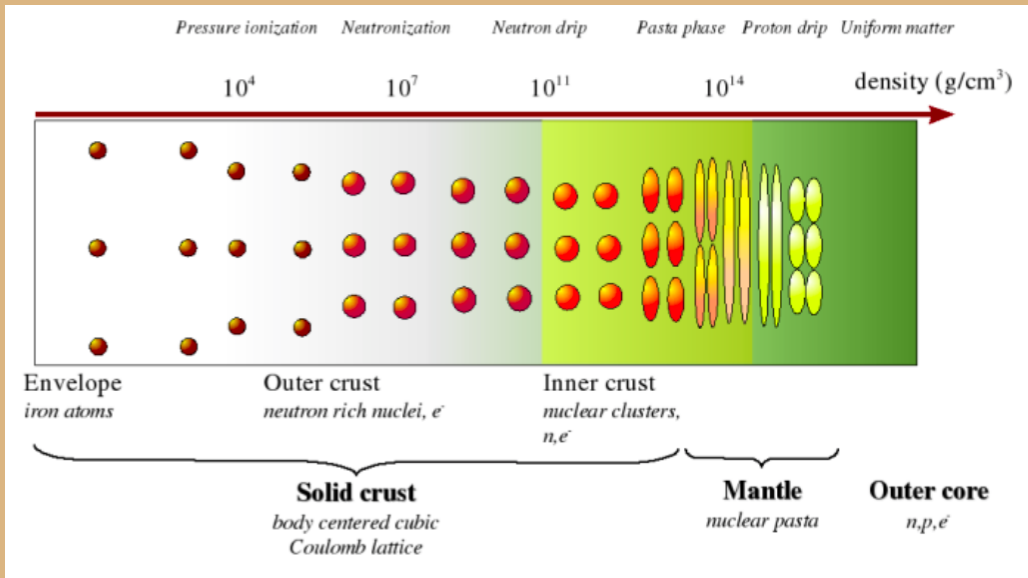


Neutron star crusts inhomogeneous

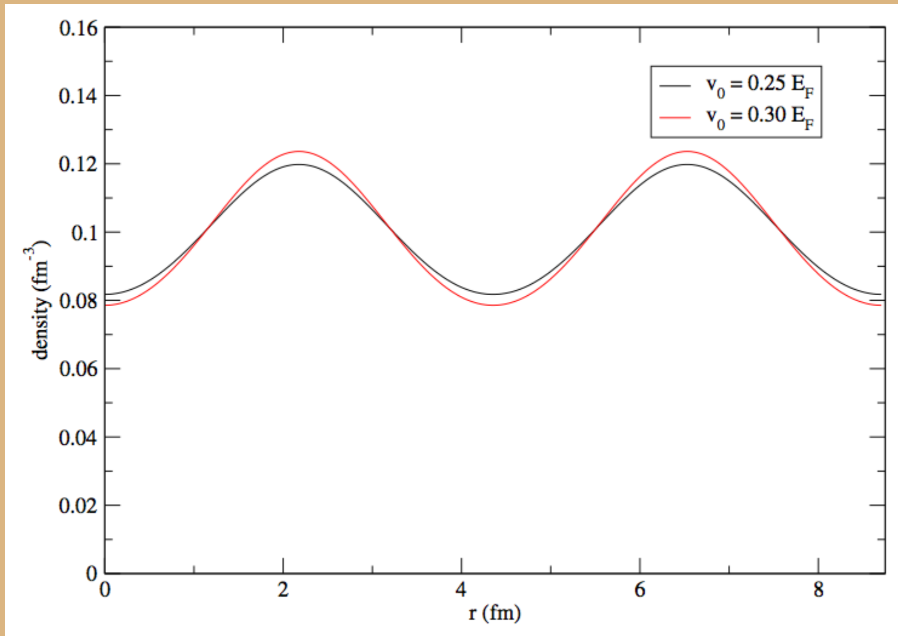




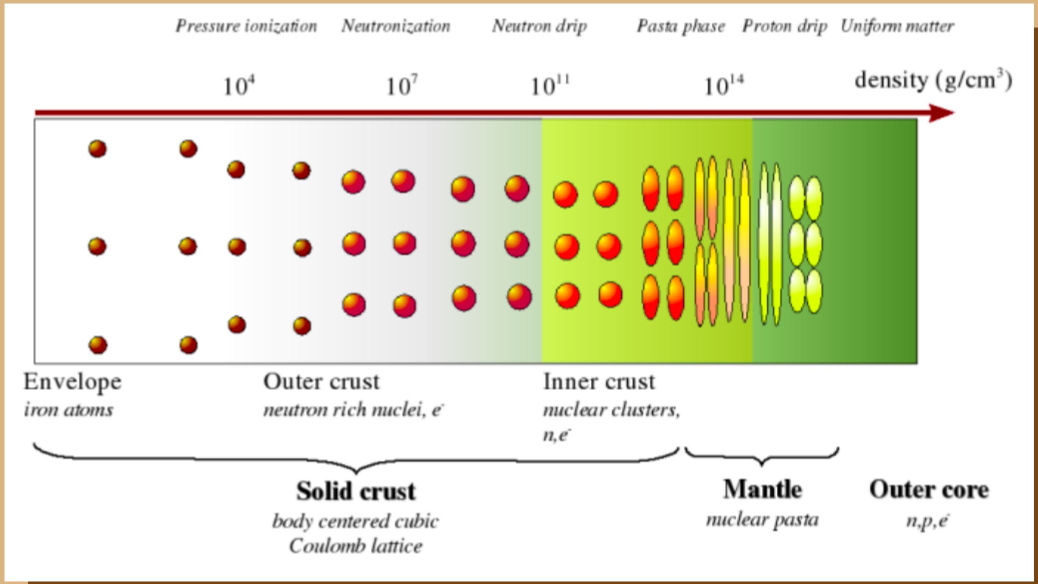
Neutron star crusts inhomogeneous



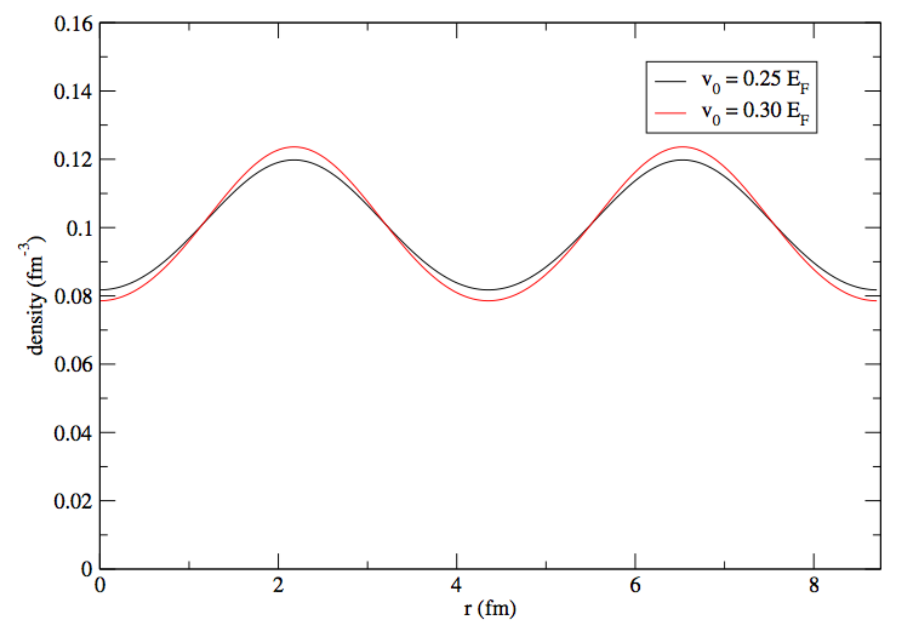
M. Buraczynski and A. Gezerlis,
Phys. Rev. Lett. **116**, 152501 (2016);
Phys. Rev. C **95**, 034012 (2017)



Neutron star crusts inhomogeneous



Situation identical to electrons in solids or atoms in optical lattices



M. Buraczynski and A. Gezerlis, Phys. Rev. Lett. **116**, 152501 (2016); Phys. Rev. C **95**, 034012 (2017)

Problem setup

Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \sum_i 2v_q \cos(\mathbf{q}\cdot\mathbf{r}_i)$$

non-relativistic kinetic energy

two-nucleon interaction

three-nucleon interaction

single-particle external potential

Problem setup

Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \sum_i 2v_q \cos(\mathbf{q}\cdot\mathbf{r}_i)$$

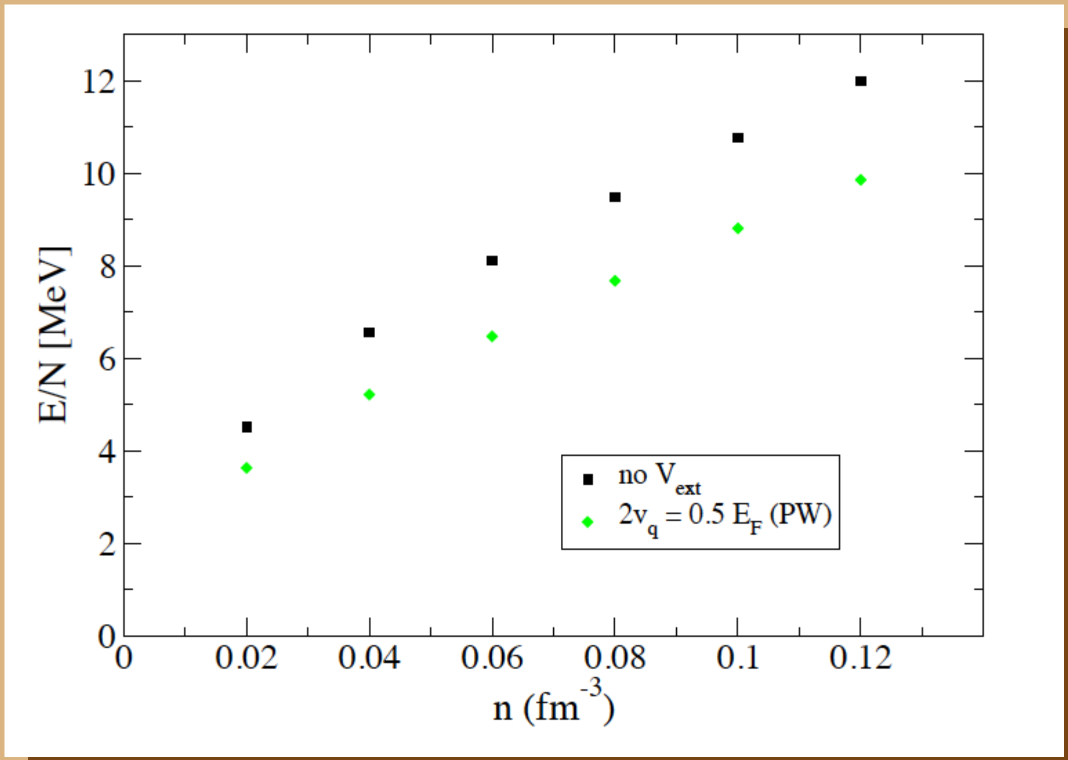
Trial wave function

$$|\Psi_T\rangle = \prod_{i<j} f(r_{ij})\ \mathcal{A}\left[\prod_i |\phi_i, s_i\rangle\right]$$

single-particle orbitals:
- plane waves
- Mathieu functions

Approach: Carry out microscopic QMC calculations for ~100 particles

One periodicity, one strength

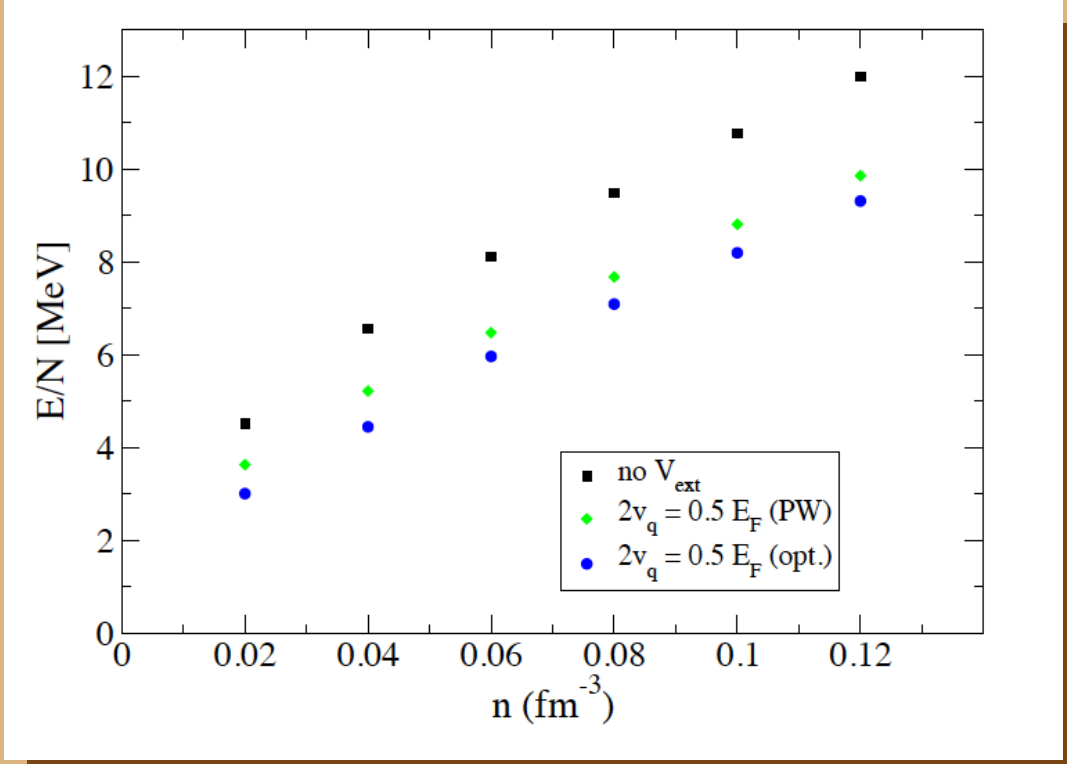


- Periodic potential in addition to nuclear forces
- Energy trivially decreased

M. Buraczynski and A. Gezerlis,
Phys. Rev. Lett. **116**, 152501 (2016)

NEUTRONS

One periodicity, one strength



- Periodic potential in addition to nuclear forces
- Energy trivially decreased
- Considerable dependence on wave function (physics input)
- Microscopic input for energy-density functionals

M. Buraczynski and A. Gezerlis,
Phys. Rev. Lett. **116**, 152501 (2016)

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Background on DFT

Standard functional in PNM

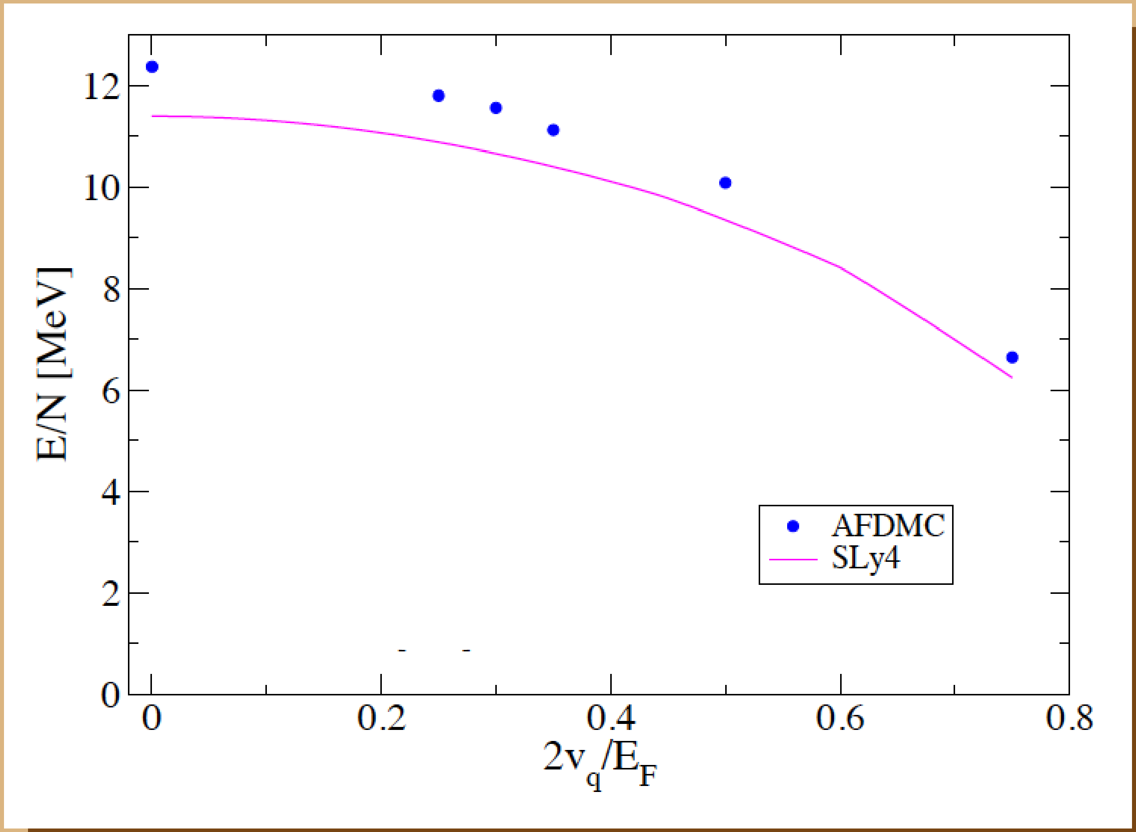
$$\mathcal{E} = \frac{\hbar^2}{2m}\tau + s_1 n^2 + s_2 n^{\sigma+2} + s_3 n\tau + s_4(\nabla n)^2$$

Skyrme functional in isospin representation

$$\mathcal{E}_{\rm Skyrme} = \sum_{T=0,1}\left[(C_T^{n,a} + C_T^{n,b} n_0^\sigma) n_T^2 + C_T^{\Delta n}(\nabla n_T)^2 + C_T^\tau n_T \tau_T\right]$$

Approach: Use QMC results to constrain DFT gradient term(s)
(which then apply to terrestrial nuclei and neutron-stars more broadly)

One periodicity, many strengths



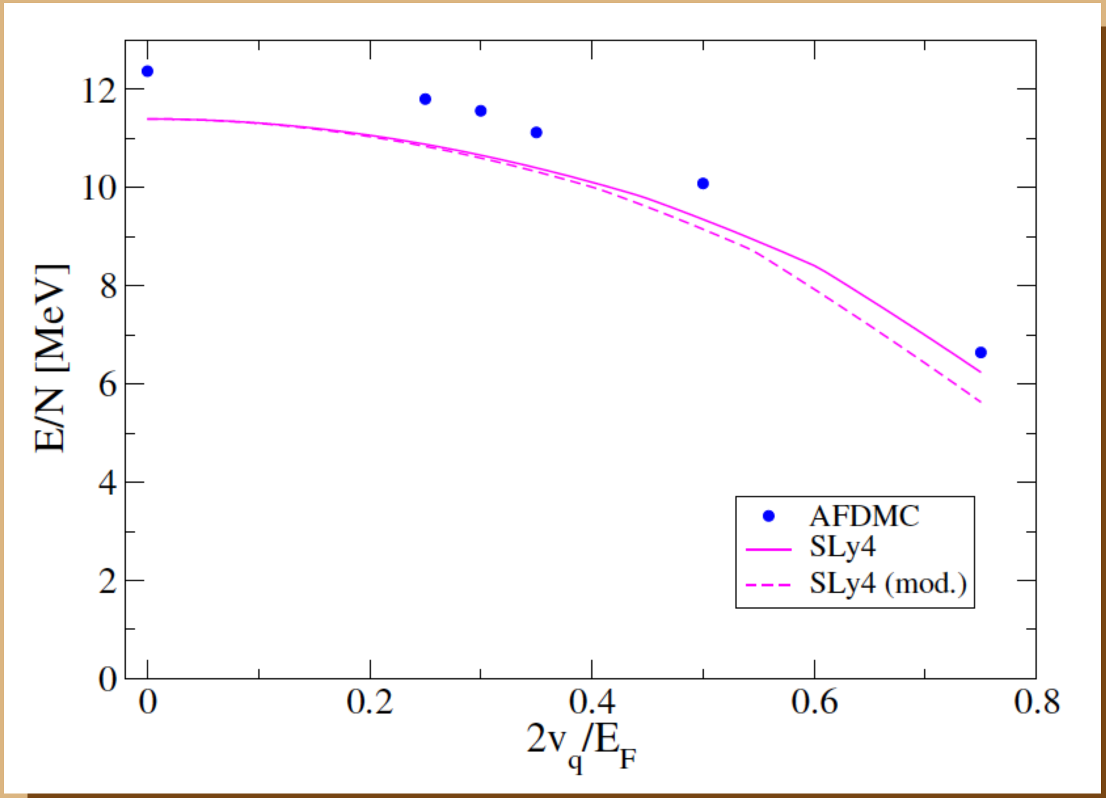
M. Buraczynski and A. Gezerlis,
Phys. Rev. Lett. **116**, 152501 (2016)

n = 0.10 fm^{-3}

- Try to disentangle bulk from isovector gradient contribution

NEUTRONS

One periodicity, many strengths



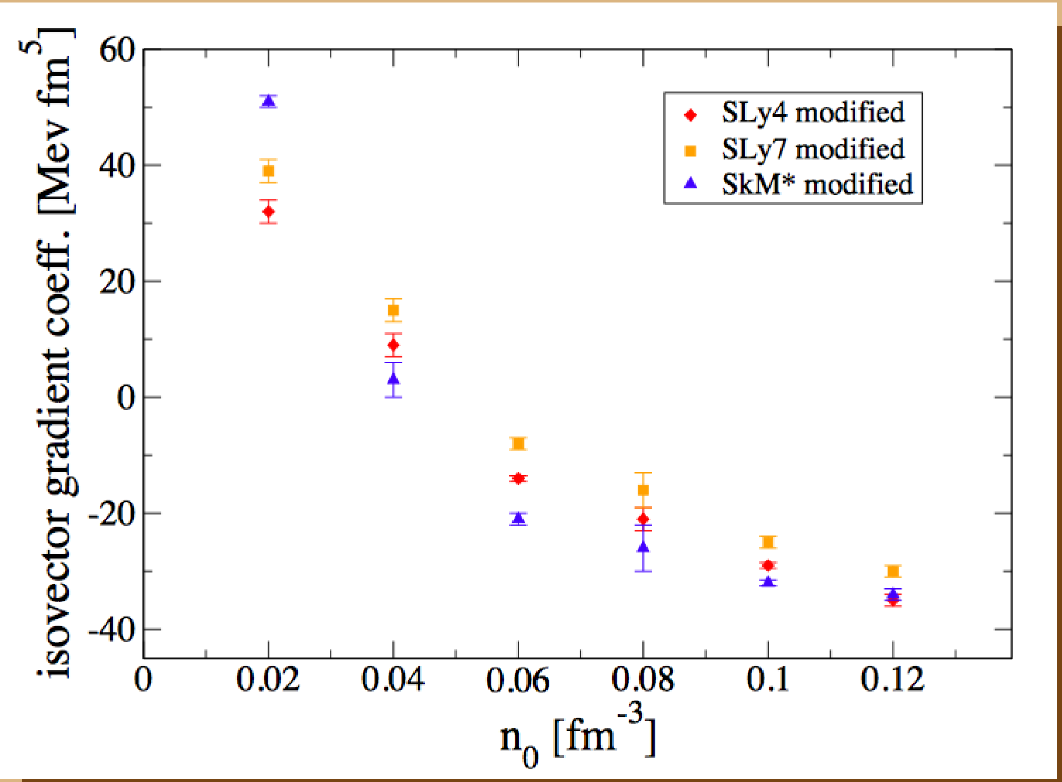
M. Buraczynski and A. Gezerlis,
Phys. Rev. Lett. **116**, 152501 (2016)

n **= 0.10 fm^{-3}**

- Try to disentangle bulk from isovector gradient contribution (homogeneous EOSs also differ)

NEUTRONS

One periodicity, many strengths



Many densities

- Repeat exercise at lower density
- Homogeneous relation is reversed
- Find density-dependent isovector coefficient, analogously to what is seen with DME (Holt, Kaiser)

NEUTRONS

M. Buraczynski and A. Gezerlis, Phys. Rev. C **95**, 034012 (2017)

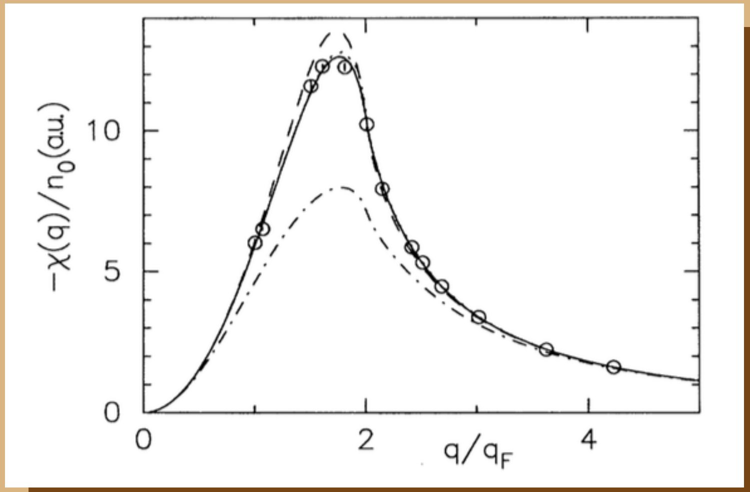
Neutron matter density response

Non-interacting gas: Lindhard function

$$\chi_L = -\frac{mq_F}{2\pi^2\hbar^2}\left[1 + \frac{q_F}{q}\left(1 - \left(\frac{q}{2q_F}\right)^2\right)\ln\left|\frac{q+2q_F}{q-2q_F}\right|\right]$$

Three-dimensional electron gas

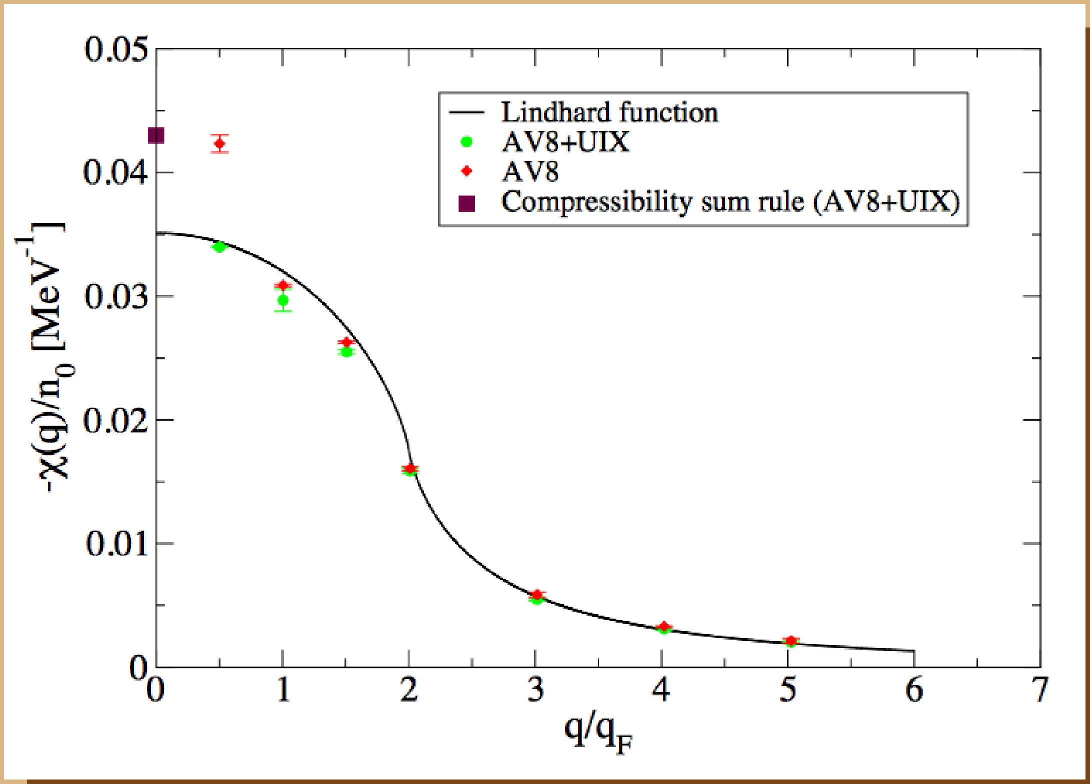
$$\frac{E_{\rm tot}}{N} = \frac{E_0}{N} + \frac{\chi(q)}{n_0}v_q^2 + C_4 v_q^4 + \cdots$$



S. Moroni, D. M. Ceperley, G. Senatore, Phys. Rev. Lett. **75**, 689 (1995)

Many periodicities, many strengths

n = 0.10 fm^{-3}



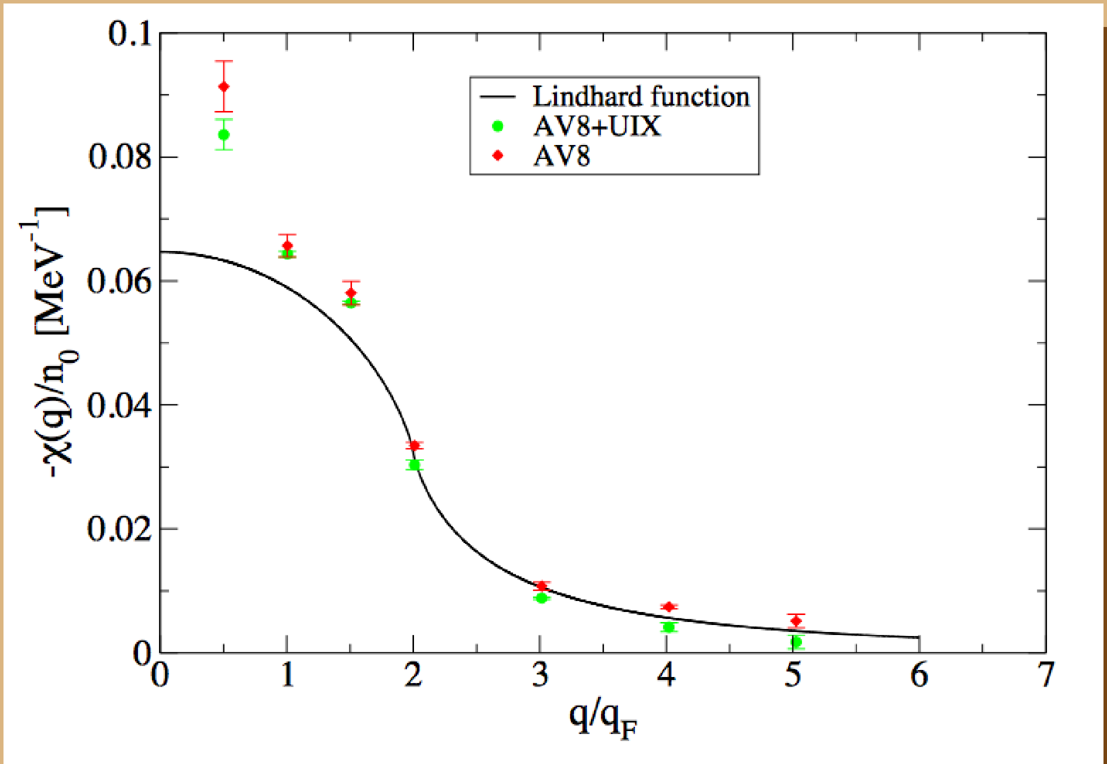
- First ever ab initio density-density response for neutron matter
- Neither Lindhard nor Coulomb
- Results on this plot derived from several strengths and periodicities

M. Buraczynski and A. Gezerlis, Phys. Rev. Lett. **116**, 152501 (2016)

M. Buraczynski and A. Gezerlis, Phys. Rev. C **95**, 034012 (2017)

NEUTRONS

Many periodicities, many strengths



$n = 0.04\ \mathrm{fm}^{-3}$

- First ever ab initio density-density response for neutron matter
- Neither Lindhard nor Coulomb
- Results on this plot derived from several strengths and periodicities

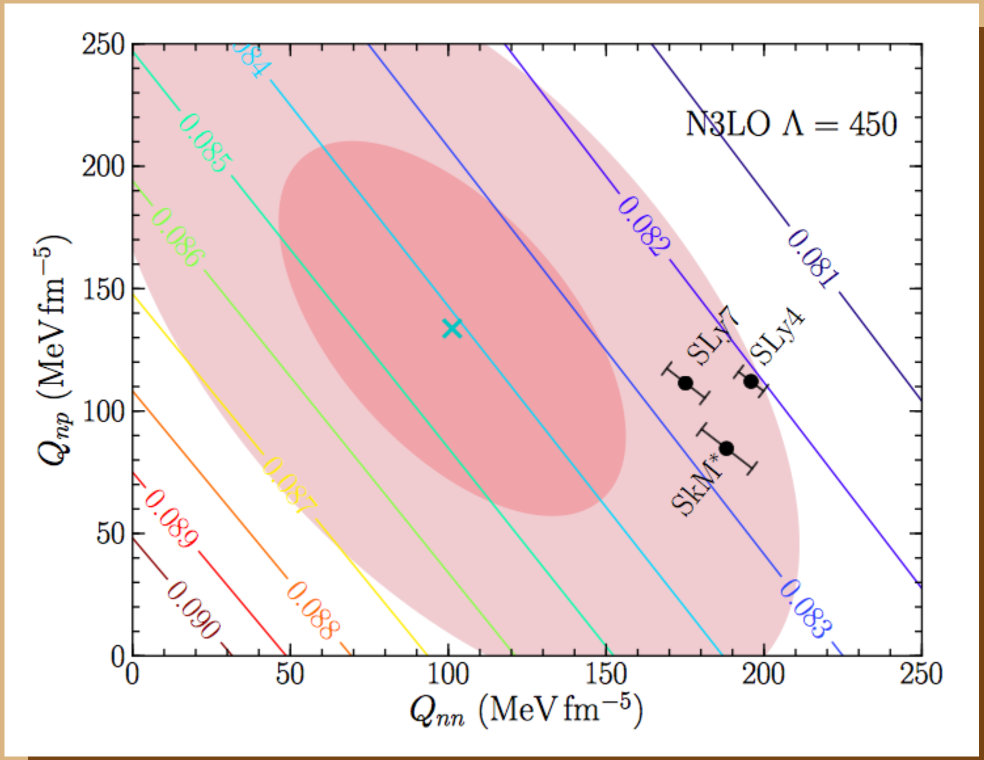
NEUTRONS

M. Buraczynski and A. Gezerlis, Phys. Rev. Lett. **116**, 152501 (2016)

M. Buraczynski and A. Gezerlis, Phys. Rev. C **95**, 034012 (2017)

Impact on neutron stars

Core-crust boundary



- Thermodynamic instability determines transition from inhomogeneous to homogeneous matter
- Modified isovector coefficients compared with large class of other results

Y. Lim and J. W. Holt, Phys. Rev. C **95**, 065805 (2017)

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

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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

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