Quantum Monte Carlo with Chiral Effective Field Theory Interactions Strongly interacting neutrons: from few to many

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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.

Quotes on degrees of freedom

"The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known**, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.**"

– Paul Dirac

"To understand macroscopic properties of matter based on understanding these microscopic laws is just unrealistic. Even though the microscopic laws are, in a strict sense, controlling what happens at the larger scale, they are not the right way to understand that."

– John Schwarz

"only a fool would imagine that one should try to understand the properties of waves in the ocean in terms of Feynman-diagram calculations in the standard model, even if the latter understanding is possible 'in principle'."

– Tom Banks

Degrees of freedom

So what does *from first principles* **mean?**

Steven Weinberg's Third Law of Progress in Theoretical Physics:

You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you'll be sorry!

Key system

Neutron stars as ultra-dense matter laboratories

- 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

Credit: Dany Page

Uncertainty estimates

Tolman-Oppenheimer-Volkoff equations (or Hartle-Thorne, etc)

Neutron stars: not just neutrons

- Indeed, mostly neutrons, but not exclusively
- Non-spherical configurations: *nuclear pasta*
- Deconfined nucleon matter throughout
- Possibly even more exotic in the core

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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

Chiral effective field theory

Nuclear interactions 3

- Attempts to connect with underlying theory (QCD)
- Systematic lowmomentum 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

Chiral EFT with Quantum Monte Carlo

Local chiral EFT

A. Gezerlis, I. Tews, E. Epelbaum, M. Freunek, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, Phys. Rev. C **90**, 054323 (2014). **A. Gezerlis**, I. Tews, E. Epelbaum, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, Phys. Rev. Lett. **111**, 032501 (2013). I. Tews, S. Gandolfi, **A. Gezerlis**, A. Schwenk, Phys. Rev. C **93**, 024305 (2016) J. E. Lynn, J. Carlson, E. Epelbaum, S. Gandolfi, **A. Gezerlis**, K. E. Schmidt, A. Schwenk, I. Tews, Phys. Rev. Lett. **113**, 192501 (2014)

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

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

Nuclear many-body problem

$H\Psi = E\Psi$

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

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

Outline

Credit: Dany Page

Motivation

Nuclear background

Main 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

M. Kortelainen et al, Phys. Rev. C **89**, 89, 054314 (2014)

Density Functional Theory

- More phenomenological (to date, but see major developments)
- Easier in crude form (orbitals \rightarrow density \rightarrow energy density)

• Can do any large N

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

Two complementary methods

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Quantum Monte Carlo Density Functional Theory

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

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

Beyond pure matter

Neutron star crusts inhomogeneous

See also: S. Moroni, D. M. Ceperley, G. Senatore, Phys. Rev. Lett. **69**, 1837 (1992); **75**, 689 (1995)

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

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

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

\n\n- plane waves
\n- Mathieu functions
\n

One periodicity, one strength

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

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

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

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

One periodicity, many strengths

Phys. Rev. Lett. **116**, 152501 (2016)

 $n = 0.10$ fm⁻³

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

Homogeneous equation of state

(homogeneous EOSs also differ)

• What about strength-dependence at different densities?

One periodicity, many strengths

NEU NEU M. Buraczynski and A. Gezerlis, *in preparation*

$$
n = 0.04
$$
 fm⁻³

- Repeat exercise at lower density
- Homogeneous relation is reversed
- Now with adjusted isovector gradient coefficient

One periodicity, many strengths

NEUTRONS M. Buraczynski and A. Gezerlis, *in preparation*

Many densities

- Find density-dependent isovector coefficient, analogously to what is seen with DME (Holt, Kaiser)
- Isovector coefficient even changes sign

Finite-size effects

Free non-interacting gas Modulated non-interacting gas

M. Buraczynski and A. Gezerlis, *in preparation*

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

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

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

M. Buraczynski and A. Gezerlis, *in preparation*

Many periodicities, many strengths

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

M. Buraczynski and A. Gezerlis, *in preparation*

Two neutrons in a finite volume

P. Klos, J. E. Lynn, I. Tews, S. Gandolfi, **A. Gezerlis**, H.-W. Hammer, M. Hoferichter, and A. Schwenk, submitted to Phys. Rev. C, arXiv:1604.01387

Lüscher's formula

$$
p \cot \delta_0(p) = \frac{1}{\pi L} S\left(\left(\frac{Lp}{2\pi}\right)^2\right)
$$

where

$$
S(\eta) = \lim_{\Lambda \to \infty} \left(\sum_{|\mathbf{j}| < \Lambda} \frac{1}{\mathbf{j}^2 - \eta} - 4\pi\Lambda \right)
$$

Combine with shape-independent approximation $p \cot \delta_0(p) = -\frac{1}{a} + \frac{1}{2}r_e p^2$

Two neutrons in a box: LO

$$
\bullet \quad q^2 = \frac{p^2 L^2}{4\pi^2}
$$

- Quantum Monte Carlo naturally suited to calculations with periodic boundary conditions
- AFDMC matches Luescher formula when pions unimportant

P. Klos, J. E. Lynn, I. Tews, S. Gandolfi, A. Gezerlis, H.-W. Hammer, M. Hoferichter, and A. Schwenk, submitted to Phys. Rev. C, arXiv:1604.01387

Lüscher's formula

Also possible to invert the process

$$
-\frac{1}{a} + \frac{1}{2}r_e p^2 = \frac{1}{\pi L}S\left(\left(\frac{Lp}{2\pi}\right)^2\right)
$$

Take results for E_i (or p_i^2) at each L_i and extract *a* and r_e

Two neutrons in a box: NLO & N²LO

$$
\bullet \quad q^2 = \frac{p^2 L^2}{4\pi^2}
$$

- Quantum Monte Carlo naturally suited to calculations with periodic boundary conditions
- Process can be inverted, to extract scattering parameters from QMC energies

P. Klos, J. E. Lynn, I. Tews, S. Gandolfi, A. Gezerlis, H.-W. Hammer, M. Hoferichter, and A. Schwenk, submitted to Phys. Rev. C, arXiv:1604.01387

General strategy

Address few-neutron systems:

- Experimental input scarce/nonexistent
- Lüscher's formula and/or handling of pions difficult

Two neutrons in a box: with cosine

NEUTRONS M. Buraczynski and A. Gezerlis, *in preparation*

- Quantum Monte Carlo naturally suited to calculations with periodic boundary conditions
- Background field easy to implement (?)

Four neutrons in a box: with cosine

NEU NEU M. Buraczynski and A. Gezerlis, *in preparation*

- Quantum Monte Carlo naturally suited to calculations with periodic boundary conditions
- Background field easy to implement (?)

Conclusions

- Rich connections between response and physics of neutron-rich nuclei, cold atoms, solid state
- 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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