Local chiral interactions for QMC simulations of matter and nuclei



Ingo Tews

Institute for Nuclear Theory Seattle & Joint Institute for Nuclear Astrophysics

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Motivation



First neutron-star merger observed on Aug 17, 2017 :



GW170817 (100s):

- Inspiral of two neutron stars detected by LIGO/VIRGO
- Distance d=40 Mpc.

GRB 170817A (2s):

- Gamma-ray burst detected by Fermi and INTEGRAL
- 2s after the merger signal.

AT 2017gfo:

- Optical transient detected 11 hours after merger
- Multiple wavelengths observed (from radio to X-ray)
- Confirmed mergers as r-process location.

First multimessenger observation!

Motivation



First neutron-star merger observed on Aug 17, 2017 :



LIGO/VIRGO collaboration, ApJL 848, L12 (2017)

Optical and near-infrared images.

- Gravitational waves probe Equation of State (EOS) e.g., Bauswein et al.
- Lightcurves probe composition of ejecta and r-process pathway Kasen et al. ApJ (2013)
- > Depend on nuclear structure close to the dripline, which will be probed at FRIB.

First multimessenger observation!

Motivation



Present theoretical predictions for nuclear systems are limited by:

- > our understanding of nuclear interactions,
- and our ability to reliably calculate these strongly interacting systems.



For nucleonic matter and nuclei, we need a consistent approach with:

- > a systematic theory for strong interactions
- advanced many-body methods
- controlled theoretical uncertainty estimates.
- Precision studies of nucleonic matter and nuclei using QMC and chiral EFT.

Outline



> What are the fundamental interactions that govern strongly interacting matter?

Chiral effective field theory: e.g. Epelbaum *et al.*, PPNP (2006) and RMP (2009)

• Systematic basis for nuclear forces, naturally includes many-body forces. Quantum Monte Carlo methods and local chiral interactions.

Gezerlis, IT, et al., PRL & PRC (2013, 2014, 2016), Lynn et al., PRL & PRC (2016, 2017), Huth et al. (2017)

> How does subatomic matter organize itself?

Results of Quantum Monte Carlo calculations with chiral interactions

- for neutron matter,
- for light to medium-mass nuclei.

> How can we understand astrophysical phenomena?

Results for astrophysical applications:.

- Neutron-star equation of state and structure.
- Neutron-star mergers

Summary.

Chiral effective field theory for nuclear forces





See talks by Kai Hebeler, Stefano Gandolfi. Systematic expansion of nuclear forces in Q over breakdown scale $\Lambda_{\rm b}$:

- Pions and nucleons as explicit degrees of freedom
- Power counting scheme
- Can work to desired accuracy with systematic error estimates
- > Natural hierarchy of nuclear forces
- Consistent interactions: Same couplings for two-nucleon and many-body sector
- Fitting: NN forces in NN system (NN phase shifts), 3N forces in 3N/4N system (Binding energies, radii)

Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Machleidt, Meißner, Hammer ...

Chiral effective field theory for nuclear forces





See also Carlsson et al. PRX (2016)

Quantum Monte Carlo method



Cast many-body Schrödinger equation as diffusion equation:

$$\lim_{\tau \to \infty} e^{-H\tau} |\Psi_T\rangle \to |\Psi_0\rangle$$
$$\psi(R,\tau) = \int dR'^{3N} \langle R|e^{-(T+V)\tau}|R'\rangle \psi(R',0)$$

Basic steps:

- ➤ Choose trial wavefunction which overlaps with the ground state $|\psi(R,0)\rangle = |\psi_T(R,0)\rangle = \sum_i c_i |\phi_i\rangle \rightarrow \sum_i c_i e^{-(E_i - E_0)\tau} |\phi_i\rangle$
- \succ Evaluate propagator for small timestep $\Delta \tau$, in practice only for local potentials
- Make consecutive small time steps using Monte Carlo techniques to project out ground state

$$|\psi_T(R,\tau)\rangle \rightarrow |\phi_0\rangle \quad \text{for} \quad \tau \rightarrow \infty$$

More details:

Carlson, Gandolfi, Pederiva, Pieper, Schiavilla, Schmidt, Wiringa, RMP (2015)

Quantum Monte Carlo method





- Very precise method for strongly interacting systems.
- With transient estimates, stochastically exact.
- > Needs as input local interactions but chiral EFT generally nonlocal!

Perturbativeness of chiral interactions





Quantum Monte Carlo: can also treat hard interactions!

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$\begin{array}{l} \blacktriangleright \quad \mbox{Pion exchanges local} \\ V_{\rm long}(r) = V_C(r) + W_C(r) \ \tau_1 \cdot \tau_2 \\ + \left(V_S(r) + W_S(r) \ \tau_1 \cdot \tau_2\right) \ \sigma_1 \cdot \sigma_2 \\ + \left(V_T(r) + W_T(r) \ \tau_1 \cdot \tau_2\right) S_{12} \end{array}$

\rightarrow local regulator

$$V_{\text{long}}(r) \rightarrow V_{\text{long}}(r) \left(1 - e^{-(r/R_0)^4}\right)$$

Contact potential:

$$V_{\text{cont}}^{(0)} = \alpha_1 \mathbf{1} + \alpha_2 \,\sigma_1 \cdot \sigma_2 + \alpha_3 \,\tau_1 \cdot \tau_2 + \alpha_4 \,\sigma_1 \cdot \sigma_2 \,\tau_1 \cdot \tau_2$$

→ Only two independent (Pauli principle)

$$V_{\text{cont}}^{(0)} = C_S 1 + C_T \sigma_1 \cdot \sigma_2$$

$$\delta(\mathbf{r}) \rightarrow \delta_{R_0}(\mathbf{r}) = \alpha e^{-(r/R_0)^4}$$



Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Machleidt, Meißner, Hammer ...





Choose local set of short-range operators at NLO (7 out of 14)

$$V_{\text{cont}}^{(2)} = \begin{array}{l} \gamma_1 q^2 + \gamma_2 q^2 \sigma_1 \cdot \sigma_2 + \gamma_3 q^2 \tau_1 \cdot \tau_2 \\ + \gamma_4 q^2 \sigma_1 \cdot \sigma_2 \tau_1 \cdot \tau_2 \\ + \gamma_5 k^2 + \gamma_6 k^2 \sigma_1 \cdot \sigma_2 + \gamma_7 k^2 \tau_1 \cdot \tau_2 \\ + \gamma_8 k^2 \sigma_1 \cdot \sigma_2 \tau_1 \cdot \tau_2 \\ + \gamma_9 (\sigma_1 + \sigma_2) (\mathbf{q} \times \mathbf{k}) \\ + \gamma_{10} (\sigma_1 + \sigma_2) (\mathbf{q} \times \mathbf{k}) \tau_1 \cdot \tau_2 \\ + \gamma_{11} (\sigma_1 \cdot \mathbf{q}) (\sigma_2 \cdot \mathbf{q}) \\ + \gamma_{12} (\sigma_1 \cdot \mathbf{q}) (\sigma_2 \cdot \mathbf{q}) \tau_1 \cdot \tau_2 \\ + \gamma_{13} (\sigma_1 \cdot \mathbf{k}) (\sigma_2 \cdot \mathbf{k}) \\ + \gamma_{14} (\sigma_1 \cdot \mathbf{k}) (\sigma_2 \cdot \mathbf{k}) \tau_1 \cdot \tau_2 \end{array}$$

Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Machleidt, Meißner, Hammer ...





Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Machleidt, Meißner, Hammer ...

- Choose local set of short-range operators at NLO (7 out of 14)
- Pion exchanges up to N²LO are local
- This freedom can be used to remove all nonlocal operators up to N²LO

Gezerlis, IT, Epelbaum, Gandolfi, Hebeler, Nogga, Schwenk, PRL (2013) Gezerlis, IT, Epelbaum, Freunek, Gandolfi, Hebeler, Nogga, Schwenk, PRC (2014)

LECs fit to phase shifts



Contact potential at LO:

$$V_{\rm cont}^{(0)} = C_1 \mathbf{1} + C_{\sigma} \sigma_{12} + C_{\tau} \tau_{12} + C_{\sigma\tau} \sigma_{12} \tau_{12}$$

Construct antisymmetrized potential:

$$V_{\rm as}(\mathbf{q}, \mathbf{k}) = \frac{1}{2} \left(V(\mathbf{q}, \mathbf{k}) - \mathcal{A}[V(\mathbf{q}, \mathbf{k})] \right)$$
$$\mathcal{A}[V(\mathbf{q}, \mathbf{k})] = \frac{1}{4} (1 + \sigma_{12})(1 + \tau_{12})V\left(\mathbf{q} \rightarrow -2\mathbf{k}, \mathbf{k} \rightarrow -\frac{1}{2}\mathbf{q}\right)$$

$$V_{\text{cont,as}}^{(0)} = \frac{1}{2} \left(1 - \frac{1}{4} (1 + \sigma_{12}) (1 + \tau_{12}) \right) V_{\text{cont}}^{(0)}$$
$$= \tilde{C}_{S} + \tilde{C}_{T} \sigma_{12} + \left(-\frac{2}{3} \tilde{C}_{S} - \tilde{C}_{T} \right) \tau_{12} + \left(-\frac{1}{3} \tilde{C}_{S} \right) \sigma_{12} \tau_{12}$$

Only two linearly independent contact interactions!



True, only when regulator f behaves like

$$f(\mathbf{q}, \mathbf{k}) = f\left(-2\mathbf{k}, -\frac{1}{2}\mathbf{q}\right)$$

but not for local regulator $f(\mathbf{q})$:

$$V_{\text{cont,as}}^{(0,\text{loc})} = \tilde{C}_{S} + \tilde{C}_{T}\sigma_{12} + \left(-\frac{2}{3}\tilde{C}_{S} - \tilde{C}_{T}\right)\tau_{12} + \left(-\frac{1}{3}\tilde{C}_{S}\right)\sigma_{12}\tau_{12} + V_{\text{corr}}^{f}(\mathbf{p}\cdot\mathbf{p}')$$

Manifestation of the fact that introducing a regulator function affects potential terms beyond the order at which one is working, and should be corrected at higher order.

But:

Violation of Fierz ambiguity can lead to sizable contributions in 3N sector. Lynn, IT, et al., PRL (2016), Dyhdalo, Hebeler, Furnstahl, IT, PRC (2016)

Leads to mixing of different partial waves.





Violation of Fierz ambiguity sizable in the NN sector at LO but restored to a large extent by including subleading operators at NLO.

> In 3N sector, subleading corrections only at N⁴LO.



Cutoff $R_0 = 1.0$ fm: Huth, IT, et al., PRC (2017)



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Local chiral interactions





Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Machleidt, Meißner, Hammer ...

- Pion exchanges up to N²LO are local
- It is possible to remove all nonlocal operators up to N²LO Gezerlis, IT, et al., PRL (2013), PRC (2014)
- > So far: cutoff variation R_0 =1.0-1.2 fm
- Two-body LECs fit to phase shifts
- Inclusion of leading 3N forces:



3N LECS fit to uncorrelated observables:

- Probe properties of light nuclei: ⁴He E_B
- > Probe spin-orbit splitting: $n-\alpha$ scattering

QMC with chiral 3N forces





 c_1, c_3, c_4



Two-pion-exchange:

- c₁ term: Tucson-Melbourn S-wave interaction
- c_{3,4} term: Fujita-Miyazawa interaction

Usually only contribution to pure neutron matter.

> Usually V_D and V_E vanish in T=3/2 or S=3/2 systems:

- V_D due to spin-isospin structure
- V_E due to Pauli principle see also Hebeler, Schwenk, PRC (2010)



Only true for regulator symmetric in particle labels like commonly used nonlocal regulators, not for local regulators!

local 3N, see also Navratil, Few Body Syst. (2007)

QMC with chiral 3N forces





 \blacktriangleright For local regulator also V_E contributes to neutron matter:

$$V_E \sim c_E \sum_{i < j < k} \sum_{\text{cyc}} \mathcal{O}_{ijk} \,\delta_{R_{3N}}(r_{ij}) \,\delta_{R_{3N}}(r_{kj})$$

Fierz ambiguity:

$$\mathcal{O}_{ijk} = \{\mathbb{1}, \, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, \, \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j, \, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j, \\ \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k, \, [(\boldsymbol{\sigma}_i \times \boldsymbol{\sigma}_j) \cdot \boldsymbol{\sigma}_k] [(\boldsymbol{\tau}_i \times \boldsymbol{\tau}_j) \cdot \boldsymbol{\tau}_k] \}.$$
Epelbaum, et al., PRC (2002)

No Fierz rearrangement freedom for local regulators, choose different short-range structures to estimate the impact:

$$V_{E\tau} \sim \tau_i \cdot \tau_j$$
$$V_{E\mathbb{1}} \sim \mathbb{1}$$
$$V_{E\mathcal{P}} \sim \mathcal{P}_{S=1/2, T=1/2}$$

See also Lovato et al. PRC (2012)



Fit c_{E} and c_{D} to ⁴He binding energy and $n-\alpha$ scattering (A \leq 5)



Lynn, IT, et al., PRL (2016)

Results





- ➤ Chiral interactions at N²LO simultaneously reproduce the properties of A≤5 systems and of neutron matter (uncertainty estimate as in E. Epelbaum et al, EPJ (2015)).
- Commonly used phenomenological 3N interactions fail for neutron matter. Sarsa, Fantoni, Schmidt, Pederiva, PRC (2003)



Results for AFDMC calculations of heavier systems ($R_0 = 1.0$ fm):

(Using the same local chiral interactions)





Results for AFDMC calculations of heavier systems ($R_0 = 1.0$ fm):

(Using the same local chiral interactions)





Results for AFDMC calculations of heavier systems ($R_0 = 1.2$ fm):

(Using the same local chiral interactions)





Results for AFDMC calculations of heavier systems ($R_0 = 1.0$ fm):

(Using the same local chiral interactions)





Results for AFDMC calculations of heavier systems ($R_0 = 1.2$ fm):

(Using the same local chiral interactions)







Piarulli et al., PRL (2018)

To-Do: Currents





Derive electroweak currents consistent with local interactions. See also Park et al., Pastore et al., Kölling et al., Menendez et al., Krebs et al, Piarulli et al.

So far, there are no currents of any kind implemented in AFDMC.

Neutron Stars





- \succ Typical masses of 1.4 M_{\odot}.
- > Typical radii of 11-13 km.
- > Average density: $\approx 1.5 \rho_0$.
- May exhibit exotic phases of matter in their cores.

Neutron-star structure described by Tolman-Oppenheimer-Volkov (TOV) equations:

$$\frac{\mathrm{dP}}{\mathrm{dr}} = -\frac{Gm(r)\varepsilon(r)}{r^2} \left(1 + \frac{P(r)}{\varepsilon(r)c^2}\right) \left(1 + \frac{4\pi P(r)r^3}{m(r)c^2}\right) \left(1 - \frac{2Gm(r)}{c^2r}\right)^{-1},$$

$$\frac{\mathrm{dm}}{\mathrm{dr}} = 4\pi r^2 \varepsilon(r)$$

with equation of state (EOS).

Neutron Stars



- Neutron-matter equation of state at saturation density and above determines mass-radius relation of neutron stars (1-1 correspondence).
- Considerable uncertainty because no reliable observational constraints except $2 M_{\odot}$ stars:
 - Future observations with NICER and Advanced LIGO!



A two-solar-mass neutron star measured using Shapiro delay

P. B. Demorest¹, T. Pennucci², S. M. Ransom¹, M. S. E. Roberts³ & J. W. T. Hessels^{4,5}

(2010)

A Massive Pulsar in a (2013) Compact Relativistic Binary

John Antoniadis,* Paulo C. C. Freire, Norbert Wex, Thomas M. Tauris, Ryan S. Lynch, Marten H. van Kerkwijk, Michael Kramer, Cees Bassa, Vik S. Dhillon, Thomas Driebe, Jason W. T. Hessels, Victoria M. Kaspi, Vladislav I. Kondratiev, Norbert Langer, Thomas R. Marsh, Maura A. McLaughlin, Timothy T. Pennucci, Scott M. Ransom, Ingrid H. Stairs, Joeri van Leeuwen, Joris P. W. Verbiest, David G. Whelan



Neutron Star EOS





> Extend results to beta equilibrium (small $Y_{e,p}$) and include crust EOS

Extend to higher densities, e.g.,

- using piecewise polytropic expansion Hebeler et al., PRL (2010) and APJ (2013)
- using speed-of-sound IT, Carlson, Gandolfi, Reddy, arXiv:1801.01923
- Meta-EOS based on empirical parameters Margueron et al., PRC 97, 025805 & 025806 (2018)





IT, Carlson, Gandolfi, Reddy, arXiv:1801.01923

Kurkela et al. (2010) Bedaque & Steiner (2015) Use the speed of sound to extend EOS:



- Assume some general form for speed of sound above transition density, e.g. Gaussians, linear segments, etc.
- Sample many different curves and reconstruct EOS.
- Can easily include phase transitions.
- Loose information on degrees of freedom.

Meta-EOS based on the nuclear empirical parameters (MM-EP)





Some empirical parameters are not well constrained by nuclear physics experiments:

- Generate uncertainties in the extrapolation to high density and large isospin asymmetry.
- The impact of these uncertainties on the nuclear EOS are determined from a meta-modelling.

Margueron, Casali, Gulminelli, PRC 97, 025805 & 025806 (2018)

Assumptions





IT, Carlson, Gandolfi, Reddy, arXiv:1801.01923

Generate thousands of EOSs that:

> Are consistent with low-density results from chiral effective field theory up to 1-2 n_0 .

- Are causal ($c_s^2 \le 1$) and stable ($c_s \ge 0$ inside neutron stars).
- Support 1.9 solar-mass neutron stars.

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Comparison of models: $n_{tr} = n_0$





Chiral EFT constraint up to saturation density:

- Good agreement of different models!
- Different degrees of generalization: from nuclear degrees of freedom (black band) up to very general model with regions of softening and phase transition, etc.

Comparison of models: $n_{tr} = 2n_0$





Chiral EFT constraint up to twice saturation density:

- Good agreement of different models!
- Different degrees of generalization: from nuclear degrees of freedom (black band) up to very general model with regions of softening and phase transition, etc.

Neutron-star merger GW170817



Tidal polarizabilities from neutronstar merger,

$$Q_{ij} = -k_2 \frac{2R^5}{3G} E_{ij} \equiv \lambda E_{ij},$$

with love number k₂

$$k_{2} = \frac{8\beta^{5}}{5}(1-2\beta)^{2}[2-y_{R}+(y_{R}-1)2\beta]$$

$$\times [2\beta(6-3y_{R}+3\beta(5y_{R}-8))$$

$$+4\beta^{3}(13-11y_{R}+\beta(3y_{R}-2)+2\beta^{2}(1+y_{R}))$$

$$+3(1-2\beta)^{2}[2-y_{R}+2\beta(y_{R}-1)]\ln(1-2\beta)]^{-1}$$

Depends on neutron star structure!

LIGO observation:

 $\Lambda \bigl(1.4 \, M_\odot \bigr) \leq 800$

INSTITUTE for

NUCLEAR THEORY

Predictions based on GW170817 posterior for NS masses





LIGO/VIRGO collaboration, PRL (2017)

Study GW170817:

- Obtain tidal polarizabilities using mass distributions of GW170817.
- \blacktriangleright We do not include prior on $\overline{\Lambda}$ from LIGO observation!

Predictions based on GW170817 posterior for NS masses





Study GW170817:

- Obtain tidal polarizabilities using mass distributions of GW170817.
- \blacktriangleright We do not include prior on $\overline{\Lambda}$ from LIGO observation!

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Predictions based on GW170817 posterior for NS masses: $n_{tr}=n_0$





'Trust' nuclear physics up to saturation density:

- Large range of tidal polarizabilities allowed, depending on freedom in high-density models
- \succ In this case, GW170817 provides constraints for the EOS.

Predictions based on GW170817 posterior for NS masses: $n_{tr}=n_0$





'Trust' nuclear physics up to saturation density and enforce $\tilde{\Lambda} \leq 800$:

- Large range of tidal polarizabilities allowed, depending on freedom in high-density models
- > In this case, GW170817 provides constraints for the EOS.

Predictions based on GW170817 posterior for NS masses: n_{tr}=2n₀





'Trust' nuclear physics up to twice saturation density:

- Range of tidal polarizabilities drastically reduced, consistent for different high-density models.
- \succ EOSs fully consistent with GW170817 without information on Λ .

Summary



- QMC calculations of matter and nuclei with local chiral potentials including NN and 3N forces are a versatile and systematic approach to *ab initio* calculations of nuclei and matter.
- ➤ Chiral interactions at N²LO simultaneously reproduce the properties of A≤16 systems and of neutron matter, commonly used phenomenological 3N interactions fail.
- There is a sizable uncertainty for nuclear interactions.
- Nuclear physics input between 1-2 n_o will be directly probed in merger observations.
- Further improvements necessary to calculate nuclei and neutron-matter EOS with improved uncertainties.

> We live in exciting times!



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