# Connecting nuclear forces with properties of nuclei and neutron stars 

## Stefano Gandolfi

Los Alamos National Laboratory (LANL)

The tower of effective (field) theories and the emergence of nuclear phenomena
Espace de Structure et reactions Nucleaires Theorique
January 16-20, 2017

www.computingnuclei.org


National Energy Research Scientific Computing Center

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Emergence of properties of nuclei and neutron stars from nuclear forces

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## Outline

Part I

- Nuclei and neutron stars: reduction and emergence
- Nuclei and neutron matter with phenomenological Hamiltonians

Part II

- Nuclear interactions from chiral effective field theory
- Chiral three-body forces, "technical" issues and open questions
- Results: $A=3,4$ binding energies, neutron- ${ }^{4} \mathrm{He}$ scattering and neutron matter. Predictive power

Conclusions

From Wikipedia:
In philosophy, systems theory, science, and art, emergence is a phenomenon whereby larger entities arise through interactions among smaller or simpler entities such that the larger entities exhibit properties the smaller/simpler entities do not exhibit.

Emergence is central in theories of integrative levels and of complex systems. For instance, the phenomenon of life as studied in biology is an emergent property of chemistry and psychological phenomena emerge from the neurobiological phenomena of living things.

From Wikipedia:
Reductionism refers to several related but distinct philosophical positions regarding the connections between phenomena, or theories, "reducing" one to another, usually considered "simpler" or more "basic". The Oxford Companion to Philosophy suggests that it is "one of the most used and abused terms in the philosophical lexicon" and suggests a three part division:

1) Ontological reductionism: a belief that the whole of reality consists of a minimal number of parts
2) Methodological reductionism: the scientific attempt to provide explanation in terms of ever smaller entities
3) Theory reductionism: the suggestion that a newer theory does not replace or absorb the old, but reduces it to more basic terms.

## The Microscopic World



Is the "direction" of arrows indicating reduction vs emergence?

How do we describe nuclear systems? Degrees of freedom?


A question for the philosophers (not a claim...): Are degrees of freedom somehow describing steps or layers of reduction/emergence?

## An emergence: The deuteron



## Nuclei and neutron stars



$$
{ }^{208} \mathrm{~Pb}, \sim 10^{-15} \mathrm{~m}, 10^{-25} \mathrm{~kg}
$$


neutron star,
$\sim 10 \mathrm{Km}, 10^{30} \mathrm{~kg}\left(2 M_{\text {solar }}\right)$

## Nuclei and neutron stars



Question: Is this a huge reduction, or a magnificient emergence?

## Neutron stars

Neutron star is a wonderful "emerged' natural laboratory


- Atmosphere: atomic and plasma physics
- Crust: physics of superfluids (neutrons, vortex), solid state physics (nuclei)
- Inner crust: deformed nuclei, pasta phase
- Outer core: nuclear matter
- Inner core: hyperons? quark matter? $\pi$ or $K$ condensates?
D. Page



## Nuclei



## SciDAC UNEDF/NUCLEI

## Nuclear Hamiltonian

Model: non-relativistic nucleons interacting with an effective nucleon-nucleon force ( NN ) and three-nucleon interaction (TNI).

$$
H=-\frac{\hbar^{2}}{2 m} \sum_{i=1}^{A} \nabla_{i}^{2}+\sum_{i<j} v_{i j}+\sum_{i<j<k} V_{i j k}
$$

$v_{i j}$ NN fitted on scattering data. Sum of operators:

$$
v_{i j}=\sum O_{i j}^{p=1,8} v^{p}\left(r_{i j}\right), \quad O_{i j}^{p}=\left(1, \vec{\sigma}_{i} \cdot \vec{\sigma}_{j}, S_{i j}, \vec{L}_{i j} \cdot \vec{S}_{i j}\right) \times\left(1, \vec{\tau}_{i} \cdot \vec{\tau}_{j}\right)
$$

- NN: Argonne AV8' and AV18. NNN: Urbana UIX and IL7.
- Local chiral forces up to N²LO (Gezerlis et al. PRL (2013), PRC (2014), Lynn et al. PRL (2016)).


## Nuclear Hamiltonian



Expansion in powers of $Q / \Lambda, Q \sim 100 \mathrm{MeV}, \wedge \sim 1 \mathrm{GeV}$. Long-range physics given explicitly by pion-exchanges (no parameters). Short-range physics: contact interactions (LECs) to fit.

Three-body forces

Urbana-Illinois $V_{i j k}$ models processes like


+ short-range correlations (spin/isospin independent).

Chiral forces at $\mathrm{N}^{2} \mathrm{LO}$ :


## Nuclear Hamiltonians

Advantages:

- Argonne interactions fit phase shifts up to high energies. At $\rho=\rho_{0}$, $k_{F} \simeq 330 \mathrm{MeV}$. Two neutrons have $\mathrm{E}_{C M} \simeq 120 \mathrm{MeV}, \mathrm{E}_{L A B} \simeq 240$ $\mathrm{MeV} . \rightarrow$ accurate up to (at least) $2-3 \rho_{0}$. Provide a very good description of several observables in light nuclei.
- Interactions derived from chiral EFT can be systematically improved. Changing the cutoff probes the physics and energy scales entering into observables. They are generally softer, and make most of the calculations easier to converge.
Disadvantages:
- Phenomenological interactions are phenomenological, not clear how to improve their quality. Systematic uncertainties hard to quantify.
- Chiral interactions describe low-energy (momentum) physics. How do they work at large momenta, (i.e. e and $\nu$ scattering)?
Important to consider both and compare predictions


## Quantum Monte Carlo

Propagation in imaginary time:

$$
H \psi\left(\vec{r}_{1} \ldots \vec{r}_{N}\right)=E \psi\left(\vec{r}_{1} \ldots \vec{r}_{N}\right) \quad \psi(t)=e^{-\left(H-E_{T}\right) t} \psi(0)
$$

Ground-state extracted in the limit of $t \rightarrow \infty$.
Propagation performed by

$$
\psi(R, t)=\langle R \mid \psi(t)\rangle=\int d R^{\prime} G\left(R, R^{\prime}, t\right) \psi\left(R^{\prime}, 0\right)
$$

- Importance sampling: $G\left(R, R^{\prime}, t\right) \rightarrow G\left(R, R^{\prime}, t\right) \Psi_{I}\left(R^{\prime}\right) / \Psi_{I}(R)$
- Constrained-path approximation to control the sign problem. Unconstrained-path calculation possible in several cases (exact).

GFMC includes all spin-states of nucleons in the w.f., nuclei up to $A=12$ AFDMC samples spin states, bigger systems, less accurate than GFMC

Ground-state obtained in a non-perturbative way. Systematic uncertainties within 1-2 \%.

## Light nuclei spectrum computed with GFMC



Carlson, Gandolfi, Pederiva, Pieper, Schiavilla, Schmidt, Wiringa, RMP (2015)
Also radii, densities, matrix elements, ...

## Neutron matter and the crisis of three-body forces



Note: AV8'+UIX and AV8' are stiff enough to support observed neutron stars. AV8' + IL7 too soft. $\rightarrow$ How to reconcile with nuclei???

## Neutron matter and the crisis of the three-body force

Extended Data Table 2| Key observables from chiral interactions. Predictions for ${ }^{48} \mathrm{Ca}$ (based on the interactions used in this work): binding energy $B E$, neutron separation energy $S_{\mathrm{n}}$, three-point-mass difference $\Delta$, electric-charge radius $R_{\mathrm{ch}}$, and the weak-charge radius $R_{\mathrm{W}}$. The last two columns show the symmetry energy of the nuclear equation of state and its slope $L$ at saturation density. Energies are in MeV and radii in fm . Theoretical uncertainty estimates are about $1 \%$ for radii and energies.

| Interaction | $B E$ | $S_{\mathrm{n}}$ | $\Delta$ | $R_{\text {ch }}$ | $R_{\mathrm{W}}$ | $S_{v}$ | $L$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| NNLO $_{\text {st }}$ | 404 | 9.5 | 2.69 | 3.48 | 3.65 | 26.9 | 40.8 |
| $1.8 / 2.0$ (EM) | 420 | 10.1 | 2.69 | 3.30 | 3.47 | 33.3 | 48.6 |
| $2.0 / 2.0$ (EM) | 396 | 9.3 | 2.66 | 3.34 | 3.52 | 31.4 | 46.7 |
| $2.2 / 2.0$ (EM) | 379 | 8.8 | 2.61 | 3.37 | 3.55 | 30.2 | 45.5 |
| $2.8 / 2.0$ (EM) | 351 | 8.0 | 2.41 | 3.44 | 3.62 | 28.5 | 43.8 |
| $2.0 / 2.0$ (PWA) | 346 | 7.8 | 2.82 | 3.55 | 3.72 | 27.4 | 44.0 |
| Experiment | 415.99 | 9.995 | 2.399 | 3.477 |  |  |  |

Hagen, et al., Nature Physics (2016)
Similar trend: very low symmetry energies, soft EOS, probably leading too small radii in neutron stars.

## Neutron matter equation of state

- Nucleon-nucleon interactions well constrained.
- The three-neutron force ( $T=3 / 2$ ) very weak in light nuclei, while $T=1 / 2$ is the dominant part.
No direct $T=3 / 2$ experiments available.
- EOS of neutron matter gives the symmetry energy and its slope.
- Determines radii of neutron stars.



## What is the Symmetry energy?



Assumption from experiments:

$$
E_{S N M}\left(\rho_{0}\right)=-16 \mathrm{MeV}, \quad \rho_{0}=0.16 \mathrm{fm}^{-3}, \quad E_{\text {sym }}=E_{P N M}\left(\rho_{0}\right)+16
$$

At $\rho_{0}$ we access $E_{\text {sym }}$ by studying PNM.

## Neutron matter

Equation of state of neutron matter using the $\mathrm{AV}^{\prime}$ + + UIX Hamiltonian.


Incidentally these can be considered as "extremes" with respect to the measured $E_{\text {sym }}$.

## Neutron matter

We consider different forms of three-neutron interaction by only requiring a particular value of $E_{\text {sym }}$ at saturation.


## Neutron matter

Equation of state of neutron matter using Argonne forces:


## Neutron matter and symmetry energy

From the EOS, we can fit the symmetry energy around $\rho_{0}$ using

$$
E_{\text {sym }}(\rho)=E_{\text {sym }}+\frac{L}{3} \frac{\rho-0.16}{0.16}+\cdots \quad\left(\text { often } \mathrm{E}_{\text {sym }} \text { called } \mathrm{S}_{0}\right)
$$



Gandolfi et al., EPJ (2014)


Lattimer, Steiner, EPJ (2014)
Very weak dependence to the model of 3 N force for a given $E_{\text {sym }}$. Chiral interactions give similar results.

## Neutron matter and neutron star structure

TOV equations:

$$
\begin{gathered}
\frac{d P}{d r}=-\frac{G\left[m(r)+4 \pi r^{3} P / c^{2}\right]\left[\epsilon+P / c^{2}\right]}{r\left[r-2 G m(r) / c^{2}\right]}, \\
\frac{d m(r)}{d r}=4 \pi \epsilon r^{2},
\end{gathered}
$$


J. Lattimer

## Neutron star structure

EOS used to solve the TOV equations.


Gandolfi, Carlson, Reddy, PRC (2012).
Accurate measurement of $E_{\text {sym }}$ put a constraint to the radius of neutron stars, OR observation of M and R would constrain $E_{\text {sym }}$ !

## Chiral three-body forces, issue (I)



For a finite cutoff, there are "additional" $V_{D}$ and $V_{E}$ diagrams coming from Fourier transforming $2 \pi$ exchange.
Usually they are effectively reabsorbed trough the fit of $c_{D}$ and $c_{E}$, but often neglected in existing neutron matter calculations.

## Neutron matter with chiral forces

Contribution of the "additional" $V_{D}$ and $V_{E}$ terms, with $c_{D}=\mathrm{c}_{E}=0$. AFDMC calculations.


Note: Contribution of FM ( $2 \pi$ exchange) about 0.9 MeV with AV8'+UIX.

## Neutron matter with chiral forces

Exploring the form of the regulator and the cutoff:


Tews, Gandolfi, Gezerlis, Schwenk, PRC (2016)

Equation of state of neutron matter at $\mathrm{N}^{2} \mathrm{LO}$.


Note: $\mathrm{c}_{D}=\mathrm{C}_{E}=0$ (they will be non-zero in a few slides).

## Chiral three-body forces, issue (II)



In the Fourier transformation of $V_{D}$ two possible operator structures arise:
$V_{D 1}=\frac{g_{A} c_{D} m_{\pi}^{2}}{96 \pi \Lambda_{\chi} F_{\pi}^{4}} \sum_{i<j<k} \sum_{c y c} \tau_{i} \cdot \tau_{k}\left[X_{i k}\left(r_{k j}\right) \delta\left(r_{i j}\right)+X_{i k}\left(r_{i j}\right) \delta\left(r_{k j}\right)-\frac{8 \pi}{m_{\pi}^{2}} \sigma_{i} \cdot \sigma_{k} \delta\left(r_{i j}\right) \delta\left(r_{k j}\right)\right]$
$V_{D 2}=\frac{g_{A} C_{D} m_{\pi}^{2}}{96 \pi \Lambda_{\chi} F_{\pi}^{4}} \sum_{i<j<k} \sum_{c y c} \tau_{i} \cdot \tau_{k}\left[X_{i k}\left(r_{i k}\right)-\frac{4 \pi}{m_{\pi}^{2}} \sigma_{i} \cdot \sigma_{k} \delta\left(r_{i k}\right)\right]\left[\delta\left(r_{i j}\right)+\delta\left(r_{k j}\right)\right]$
$X_{i j}(r)=T(r) S_{i j}+Y(r) \sigma_{i} \cdot \sigma_{j}$
Navratil (2007), Tews et al PRC (2016), Lynn et al PRL (2016).
Equivalent only in the limit of an infinite cutoff. Implications in real life?

## Chiral three-body forces, issue (III)



Equivalent forms of operators entering in $V_{E}$ (or combinations of them):
$1, \quad \sigma_{i} \cdot \sigma_{j}, \quad \tau_{i} \cdot \tau_{j}, \quad \sigma_{i} \cdot \sigma_{j} \tau_{i} \cdot \tau_{j}, \quad \sigma_{i} \cdot \sigma_{j} \tau_{i} \cdot \tau_{k}, \quad\left[\left(\sigma_{i} \times \sigma_{j}\right) \cdot \sigma_{k}\right]\left[\left(\tau_{i} \times \tau_{j}\right) \cdot \tau_{k}\right]$
Epelbaum et al (2002). We investigated three choices:

$$
\begin{aligned}
& V_{E \tau}=\frac{c_{E}}{\Lambda_{\chi} F_{\pi}^{4}} \sum_{i<j<k} \sum_{\text {cyc }} \tau_{i} \cdot \tau_{k} \delta\left(r_{k j}\right) \delta\left(r_{i j}\right) \\
& V_{E 1}=\frac{c_{E}}{\Lambda_{\chi} F_{\pi}^{4}} \sum_{i<j<k} \sum_{\mathrm{cyc}} \delta\left(r_{k j}\right) \delta\left(r_{i j}\right) \\
& V_{E \mathcal{P}}=\frac{c_{E}}{\Lambda_{\chi} F_{\pi}^{4}} \sum_{i<j<k} \sum_{\mathrm{cyc}} \mathcal{P}_{S, T=1 / 2} \delta\left(r_{k j}\right) \delta\left(r_{i j}\right)
\end{aligned}
$$

Qualitative differences expected, i.e. consider ${ }^{4} \mathrm{He}$ vs, neutron』matter!

## Chiral three-body forces

Coefficients $c_{D}$ and $c_{E}$ fit to reproduce the binding energy of ${ }^{4} \mathrm{He}$ and neutron- ${ }^{4} \mathrm{He}$ scattering. $\rightarrow$ more information on $\mathrm{T}=3 / 2$ part of three-body interaction.


GFMC neutron- ${ }^{4} \mathrm{He}$ results using Argonne Hamiltonians.

Nollett, Pieper, Wiringa, Carlson, Hale, PRL (2007).

## ${ }^{4}$ He binding energy and p -wave $\mathrm{n}-{ }^{4}$ He scattering

Regulator: $\delta(r)=\frac{1}{\pi \Gamma(3 / 4) R_{0}^{3}} \exp \left(-\left(r / R_{0}\right)^{4}\right)$
Cutoff $R_{0}$ taken consistently with the two-body interaction.



No fit to both observables can be obtained for $R_{0}=1.2 \mathrm{fm}$ and $V_{D 1}$
Lynn, Tews, Carlson, Gandolfi, Gezerlis, Schmidt, Schwenk PRL (2016).

## $\mathrm{A}=3,4$ nuclei at N 2 LO



Error quantification: define $Q=\max \left(\frac{p}{\Lambda_{b}}, \frac{m_{\pi}}{\Lambda_{b}}\right)$ and calculate:

$$
\Delta(N 2 L O)=\max \left(Q^{4}\left|\hat{O}_{L O}\right|, Q^{2}\left|\hat{O}_{L O}-\hat{O}_{N L O}\right|, Q \mid \hat{O}_{N L O}-\hat{O}_{N 2 L O}\right)
$$

Epelbaum, Krebs, Meissner (2014).

## Neutron matter at N2LO

EOS of pure neutron matter at $\mathrm{N} 2 \mathrm{LO}, R_{0}=1.0 \mathrm{fm}$.
Error quantification estimated as previously.



Lynn, Tews, Carlson, Gandolfi, Gezerlis, Schmidt, Schwenk PRL (2016).

- Ab-initio QMC methods useful to study nuclear systems in a coherent framework using phenomenological and local chiral forces.
- Spectrum of nuclei and other properties Argonne Hamiltonians, but problems in describing neutron matter.
- Many ambiguities regarding the choice of three-body operators. Effect in heavier nuclei and nuclear matter?
Provocation: Same issue for NN???
- (some) local chiral interaction describe $A=3,4,5$ and neutron matter.

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- Alex Gezerlis (Guelph)
- Kevin Schmidt (ASU)
- Evgeny Epelbaum (Bochum)


## Extra slides

## Scattering data and neutron matter

Two neutrons have

$$
k \approx \sqrt{E_{l a b} m / 2}, \quad \rightarrow k_{F}
$$

that correspond to

$$
k_{F} \rightarrow \rho \approx\left(E_{l a b} m / 2\right)^{3 / 2} / 2 \pi^{2} .
$$

$E_{l a b}=150 \mathrm{MeV}$ corresponds to about $0.12 \mathrm{fm}^{-3}$.
$E_{l a b}=350 \mathrm{MeV}$ to $0.44 \mathrm{fm}^{-3}$.
Argonne potentials useful to study dense matter above $\rho_{0}=0.16 \mathrm{fm}^{-3}$

## Variational wave function

$$
E_{0} \leq E=\frac{\langle\psi| H|\psi\rangle}{\langle\psi \mid \psi\rangle}=\frac{\int d r_{1} \ldots d r_{N} \psi^{*}\left(r_{1} \ldots r_{N}\right) H \psi^{*}\left(r_{1} \ldots r_{N}\right)}{\int d r_{1} \ldots d r_{N} \psi^{*}\left(r_{1} \ldots r_{N}\right) \psi^{*}\left(r_{1} \ldots r_{N}\right)}
$$

$\rightarrow$ Monte Carlo integration. Variational wave function:

$$
\left|\Psi_{T}\right\rangle=\left[\prod_{i<j} f_{c}\left(r_{i j}\right)\right]\left[\prod_{i<j<k} f_{c}\left(r_{i j k}\right)\right]\left[1+\sum_{i<j, p} \prod_{k} u_{i j k} f_{p}\left(r_{i j}\right) O_{i j}^{p}\right]|\Phi\rangle
$$

where $O^{p}$ are spin/isospin operators, $f_{c}, u_{i j k}$ and $f_{p}$ are obtained by minimizing the energy. About 30 parameters to optimize.
$|\Phi\rangle$ is a mean-field component, usually HF. Sum of many Slater determinants needed for open-shell configurations.

BCS correlations can be included using a Pfaffian.

## Quantum Monte Carlo

Propagation in imaginary time:

$$
H \psi\left(\vec{r}_{1} \ldots \vec{r}_{N}\right)=E \psi\left(\vec{r}_{1} \ldots \vec{r}_{N}\right) \quad \psi(t)=e^{-\left(H-E_{T}\right) t} \psi(0)
$$

Ground-state extracted in the limit of $t \rightarrow \infty$.
Propagation performed by

$$
\psi(R, t)=\langle R \mid \psi(t)\rangle=\int d R^{\prime} G\left(R, R^{\prime}, t\right) \psi\left(R^{\prime}, 0\right)
$$

- Importance sampling: $G\left(R, R^{\prime}, t\right) \rightarrow G\left(R, R^{\prime}, t\right) \Psi_{I}\left(R^{\prime}\right) / \Psi_{I}(R)$
- Constrained-path approximation to control the sign problem. Unconstrained-path calculation possible in several cases (exact).

GFMC includes all spin-states of nucleons in the w.f., nuclei up to $A=12$ AFDMC samples spin states, bigger systems, less accurate than GFMC

Ground-state obtained in a non-perturbative way. Systematic uncertainties within 1-2 \%.

## The Sign problem in one slide

Evolution in imaginary-time:

$$
\psi_{I}\left(R^{\prime}\right) \Psi\left(R^{\prime}, t+d t\right)=\int d R G\left(R, R^{\prime}, d t\right) \frac{\psi_{l}\left(R^{\prime}\right)}{\psi_{l}(R)} \psi_{I}(R) \Psi(R, t)
$$

note: $\Psi(R, t)$ must be positive to be "Monte Carlo" meaningful.
Fixed-node approximation: solve the problem in a restricted space where $\psi>0$ (Bosonic problem) $\Rightarrow$ upperbound.

If $\psi$ is complex:

$$
\left|\psi_{l}\left(R^{\prime}\right)\right|\left|\Psi\left(R^{\prime}, t+d t\right)\right|=\int d R G\left(R, R^{\prime}, d t\right)\left|\frac{\psi_{l}\left(R^{\prime}\right)}{\psi_{l}(R)}\right|\left|\psi_{l}(R)\right||\Psi(R, t)|
$$

Constrained-path approximation: project the wave-function to the real axis. Extra weight given by $\cos \Delta \theta$ (phase of $\left.\frac{\Psi\left(R^{\prime}\right)}{\Psi(R)}\right), \operatorname{Re}\{\Psi\}>0 \Rightarrow$ not necessarily an upperbound.

## Unconstrained-path

GFMC unconstrained-path propagation:


Changing the trial wave function gives same results.

## Unconstrained-path

AFDMC unconstrained-path propagation:


The difference between CP and UP results is mainly due to the presence of LS terms in the Hamiltonian. Same for heavier systems.

Work in progress to improve $\Psi$ to improve the constrained-path.

## Quantum Monte Carlo

$$
H \psi\left(\vec{r}_{1} \ldots \vec{r}_{N}\right)=E \psi\left(\vec{r}_{1} \ldots \vec{r}_{N}\right) \quad \psi(t)=e^{-\left(H-E_{T}\right) t} \psi(0)
$$

Ground-state extracted in the limit of $t \rightarrow \infty$.
Propagation performed by

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\psi(R, t)=\langle R \mid \psi(t)\rangle=\int d R^{\prime} G\left(R, R^{\prime}, t\right) \psi\left(R^{\prime}, 0\right)
$$

- Importance sampling: $G\left(R, R^{\prime}, t\right) \rightarrow G\left(R, R^{\prime}, t\right) \Psi_{l}\left(R^{\prime}\right) / \Psi_{l}(R)$
- Constrained-path approximation to control the sign problem. Unconstrained calculation possible in several cases (exact).

Ground-state obtained in a non-perturbative way. Systematic uncertainties within 1-2 \%.

## Overview

Recall: propagation in imaginary-time

$$
e^{-(T+V) \Delta \tau} \psi \approx e^{-T \Delta \tau} e^{-V \Delta \tau} \psi
$$

Kinetic energy is sampled as a diffusion of particles:

$$
e^{-\nabla^{2} \Delta \tau} \psi(R)=e^{-\left(R-R^{\prime}\right)^{2} / 2 \Delta \tau} \psi(R)=\psi\left(R^{\prime}\right)
$$

The (scalar) potential gives the weight of the configuration:

$$
e^{-V(R) \Delta \tau} \psi(R)=w \psi(R)
$$

Algorithm for each time-step:

- do the diffusion: $R^{\prime}=R+\xi$
- compute the weight $w$
- compute observables using the configuration $R^{\prime}$ weighted using $w$ over a trial wave function $\psi_{T}$.
For spin-dependent potentials things are much worse!


## Branching

The configuration weight $w$ is efficiently sampled using the branching technique:


Configurations are replicated or destroyed with probability

$$
\operatorname{int}[w+\xi]
$$

Note: the re-balancing is the bottleneck limiting the parallel efficiency.

Because the Hamiltonian is state dependent, all spin/isospin states of nucleons must be included in the wave-function.
Example: spin for 3 neutrons (radial parts also needed in real life):

## GFMC wave-function:

$$
\psi=\left(\begin{array}{l}
a_{\uparrow \uparrow \uparrow} \\
a_{\uparrow \uparrow \downarrow} \\
a_{\uparrow \downarrow \uparrow \uparrow} \\
a_{\uparrow \downarrow \downarrow} \\
a_{\downarrow \uparrow \uparrow} \\
a_{\downarrow \uparrow \downarrow} \\
a_{\downarrow \downarrow \uparrow} \\
a_{\downarrow \downarrow \downarrow}
\end{array}\right)
$$

A correlation like

$$
1+f(r) \sigma_{1} \cdot \sigma_{2}
$$

can be used, and the variational wave function can be very good. Any operator accurately computed.

AFDMC wave-function:

$$
\psi=\mathcal{A}\left[\xi_{s_{1}}\binom{a_{1}}{b_{1}} \xi_{s_{2}}\binom{a_{2}}{b_{2}} \xi_{s_{3}}\binom{a_{3}}{b_{3}}\right]
$$

We must change the propagator by using the Hubbard-Stratonovich transformation:

$$
e^{\frac{1}{2} \Delta t O^{2}}=\frac{1}{\sqrt{2 \pi}} \int d x e^{-\frac{x^{2}}{2}+x \sqrt{\Delta t} O}
$$

Auxiliary fields $x$ must also be sampled. The wave-function is pretty bad, but we can simulate larger systems (up to $A \approx 100$ ). Operators (except the energy) are very hard to be computed, but in some case there is some trick!

## Propagator

We first rewrite the potential as:

$$
\begin{aligned}
V & =\sum_{i<j}\left[v_{\sigma}\left(r_{i j}\right) \vec{\sigma}_{i} \cdot \vec{\sigma}_{j}+v_{t}\left(r_{i j}\right)\left(3 \vec{\sigma}_{i} \cdot \hat{r}_{i j} \vec{\sigma}_{j} \cdot \hat{r}_{i j}-\vec{\sigma}_{i} \cdot \vec{\sigma}_{j}\right)\right]= \\
& =\sum_{i, j} \sigma_{i \alpha} A_{i \alpha ; j \beta} \sigma_{j \beta}=\frac{1}{2} \sum_{n=1}^{3 N} O_{n}^{2} \lambda_{n}
\end{aligned}
$$

where the new operators are

$$
O_{n}=\sum_{j \beta} \sigma_{j \beta} \psi_{n, j \beta}
$$

Now we can use the HS transformation to do the propagation:

$$
e^{-\Delta \tau \frac{1}{2} \sum_{n} \lambda O_{n}^{2}} \psi=\prod_{n} \frac{1}{\sqrt{2 \pi}} \int d x e^{-\frac{x^{2}}{2}+\sqrt{-\lambda \Delta \tau} \times O_{n}} \psi
$$

Computational cost $\approx(3 N)^{3}$.

Three-body forces, Urbana, Illinois, and local chiral $\mathrm{N}^{2}$ LO can be exactly included in the case of neutrons.
For example:

$$
\begin{aligned}
O_{2 \pi} & =\sum_{c y c}\left[\left\{X_{i j}, X_{j k}\right\}\left\{\tau_{i} \cdot \tau_{j}, \tau_{j} \cdot \tau_{k}\right\}+\frac{1}{4}\left[X_{i j}, X_{j k}\right]\left[\tau_{i} \cdot \tau_{j}, \tau_{j} \cdot \tau_{k}\right]\right] \\
& =2 \sum_{c y c}\left\{X_{i j}, X_{j k}\right\}=\sigma_{i} \sigma_{k} f\left(r_{i}, r_{j}, r_{k}\right)
\end{aligned}
$$

The above form can be included in the AFDMC propagator.

## Neutron matter equation of state

Neutron matter is an "exotic" system. Why do we care?

- EOS of neutron matter gives the symmetry energy and its slope.
- The three-neutron force ( $T=3 / 2$ ) very weak in light nuclei, while $T=1 / 2$ is the dominant part. No direct $T=3 / 2$ experiments available.
- Determines radii of neutron stars.



## What is the Symmetry energy?



Assumption from experiments:

$$
E_{S N M}\left(\rho_{0}\right)=-16 \mathrm{MeV}, \quad \rho_{0}=0.16 \mathrm{fm}^{-3}, \quad E_{\text {sym }}=E_{P N M}\left(\rho_{0}\right)+16
$$

At $\rho_{0}$ we access $E_{\text {sym }}$ by studying PNM.

## Neutron matter

Model uncertainty vs $\mathrm{E}_{\text {sym }}$ uncertainty:


## Neutron matter and symmetry energy

From the EOS, we can fit the symmetry energy around $\rho_{0}$ using

$$
E_{\text {sym }}(\rho)=E_{\text {sym }}+\frac{L}{3} \frac{\rho-0.16}{0.16}+\cdots
$$



Gandolfi et al., EPJ (2014)


Tsang et al., PRC (2012)

Very weak dependence to the model of 3 N force for a given $E_{\text {sym }}$. Knowing $E_{\text {sym }}$ or $L$ useful to constrain 3N! (within this model...)

## Neutron star structure

EOS used to solve the TOV equations.


Gandolfi, Carlson, Reddy, PRC (2012).
Accurate measurement of $E_{\text {sym }}$ put a constraint to the radius of neutron stars, OR observation of M and R would constrain $E_{\text {sym }}$ !

## Neutron stars



Steiner, Lattimer, Brown, ApJ (2010)

Neutron star observations can be used to 'measure' the EOS and constrain $E_{\text {sym }}$ and L. (Systematic uncertainties still under debate

## Neutron star matter

Neutron star matter model:

$$
E_{N S M}=a\left(\frac{\rho}{\rho_{0}}\right)^{\alpha}+b\left(\frac{\rho}{\rho_{0}}\right)^{\beta}, \quad \rho<\rho_{t}
$$

form suggested by QMC simulations, contrast with the commonly used $E_{F G}+V$ and a high density model for $\rho>\rho_{t}$
i) two polytropes
ii) polytrope+quark matter model


Neutron star radius sensitive to the EOS at nuclear densities!
Direct way to extract $E_{\text {sym }}$ and $L$ from neutron stars observations:

$$
E_{\text {sym }}=a+b+16, \quad L=3(a \alpha+b \beta)
$$

Neutron star matter really matters!


$32<E_{\text {sym }}<34 \mathrm{MeV}$
$43<L<52 \mathrm{MeV}$
Steiner, Gandolfi, PRL (2012).

