Perspectives of ab Initio Computations of Medium/Heavy Hypernuclei

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Outline:

- Quantum Monte Carlo: what can be computed by it? What is the state of the art? What is its relevance?
- A few words on our approach to the hyperon-nucleon potential, and some (exciting) perspectives for the future.

The non relativistic many-body problem

Many problems of interest in physics can be addressed by solving a ***non-relativistic quantum problem*** *f*or *N* interacting particles:

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

where $|\Psi\rangle$ is the *N* particle state, and

$$\hat{H} = \sum_{i=0}^{N} -\frac{\hat{p}_i^2}{2m_i} + \hat{V}(1,2,3,...,N)$$

The potential can be as simple as the Coulomb potential, or as complicated as, for instance, the Argonne AV18 + UIX or some EFT nucleon-nucleon force (local or non local).

A general solution

There is an interesting, general way of solving the many-body Schroedinger problem, at least for the ground state. Let us consider the following operator, that we call "propagator"($\hbar$=*1)*:

$$e^{-(\hat{H}-E_0)\tau}$$

where E_0 is the ground state eigenvalue. If we apply it to an arbitrary state $|\Psi\rangle$ we obtain:

$$e^{-(\hat{H}-E_0)\tau}|\Psi\rangle = \sum_{n=0}^{\infty} c_n e^{-(E_n-E_0)\tau}|\Psi_n\rangle$$

where:

$$\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$$

A general solution

In the limit of large τ it is easily seen that:

$$\lim_{\tau \to \infty} e^{-(\hat{H}-E_0)\tau} |\Psi\rangle = c_0 |\Psi_0\rangle$$

provided that the initial state is not orthogonal to the ground state.

NB: This is an example within the more general class of *"power methods"*.

All this is very general: no mention is made either of the details of H or of the representation of the states.

Projection Monte Carlo algorithms are based on a ***stochastic implementation*** of this "imaginary time propagation". Different flavours correspond to the choice of a **specific representation** of the propagator and/or of the **specific Hilbert space** used.

Projection Monte Carlo

The stochastic implementation of the imaginary time propagator is made by *sampling a sequence of states* in some Hilbert space. Each state is sampled starting from the previous one with a probability given by the propagator.

For instance, if the potential depends on the coordinates of the particles only, the formulation is relatively simple. First, we approximate our state with an expansion on a finite set of points in space:

$$|\Psi\rangle \sim \sum_{i=1}^{M_w} \langle R_i|\Psi\rangle |R_i\rangle$$

Particle coordinates

$$|R_i\rangle = \delta(R - R_i) \qquad R \equiv \{\vec{r}_1 \ldots \vec{r}_N\}$$

$$\langle R|\Psi\rangle \equiv \Psi(R)$$

Wavefunction in coordinate space

AFDMC

Stefano Fantoni & Kevin Schmidt, 1999

The computational cost can be reduced in a Monte Carlo framework by introducing a way of sampling over the space of states, rather than summing explicitly over the full set.
For simplicity let us consider only one of the terms in the interaction.
We start by observing that:

Linear combination of spin operators for different particles

$$\sum_{i<j} v(r_{ij})\vec{\sigma}_i \cdot \vec{\sigma}_j = \frac{1}{2}\sum_{i;\alpha,j;\beta} \sigma_{i;\alpha} A_{i;\alpha,j;\beta}\sigma_{j;\beta} = \sum_{n=1}^{3A} \lambda_n \hat{O}_n^2$$

Then, we can linearize the operatorial dependence in the propagator by means of an integral transform:

auxiliary fields→Auxiliary Field Diffusion Monte Carlo

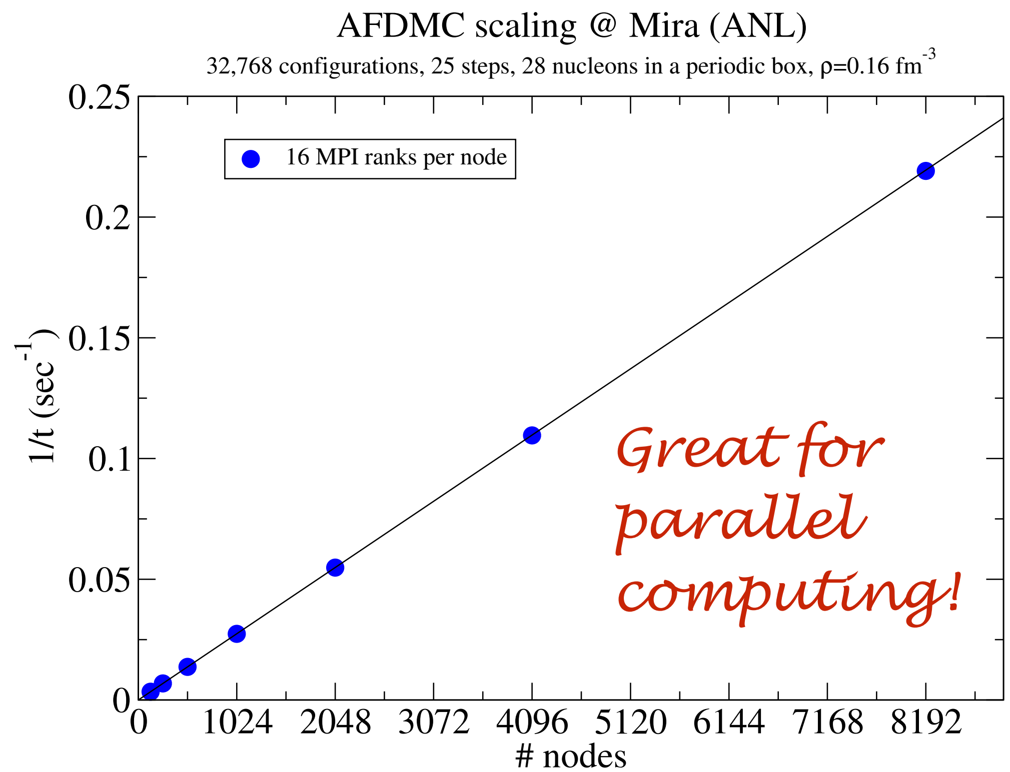
$$e^{-\frac{1}{2}\lambda \hat{O}_n^2 \Delta\tau} = \frac{1}{\sqrt{2\pi}} \int dx e^{-\frac{x^2}{2}} e^{-x\sqrt{\lambda\Delta\tau}\hat{O}_n}$$

Hubbard-Stratonovich transformation

K. E. Schmidt and S. Fantoni, Phys. Lett. B 446, 99 (1999).
S. Gandolfi, F. Pederiva, S. Fantoni, and K. E. Schmidt, Phys. Rev. Lett. 99, 022507 (2007)

AFDMC

The crucial advantage of AFDMC is that the scaling of the required computer resources is no longer exponential: **the cost scales as *A^3*** (the scaling required by the computation of the determinants in the antisymmetric wave functions) ➞ **LARGER SYSTEMS ACCESSIBLE!**



Progress

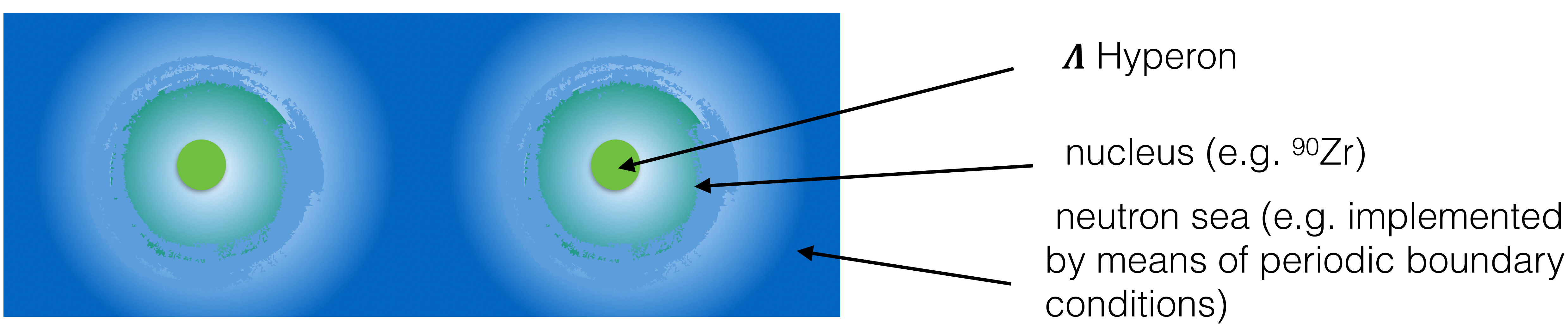
- The HS transformation can be used ONLY FOR THE PROPAGATOR Accurate wave functions require an operatorial dependence! "Cluster expansion" introduced and working!(Gandolfi, Lovato, Schmidt)
- Some problems in treating nuclear spin-orbit have been addressed.
- Three-body forces are now implemented in a quasi-perturbative way, but results are very promising.

AFDMC

What can we do?

This is a crucial question if we want to address the questions relevant for a possible hyper nuclear program at J-Lab.

- Currently we can efficiently do calculations up to A=90/91. Not all most recent improvements are implemented yet (e.g. CVMC-like variational functions). In principle the use of more realistic potentials (up to AV8') in the nucleon sector is possible, at least for checking purposes.
- We could in principle push the calculations further. For instance ^{208}Pb is computable, but with an expected use of computer time (to reach a sufficient statistics) of order 10^7 core hours. This means a **substantial investment in computational resources.**
- **"**Cheaper" models (maybe even more useful for astrophysical applications) might be based on a neutron rich matter, and compared e.g. with Pb results.



Fock space calculations

The stochastic power method can also be used in Fock space. In this case the propagator acts on the occupation number of a basis set used to span the Hilbert space of the solution of a given Hamiltonian. In particular, given two basis states $|\mathbf{m}\rangle$ and $|\mathbf{n}\rangle$ the quantity:

$$\langle \mathbf{m} | \mathcal{P}_{\Delta\tau} | \mathbf{n} \rangle = \langle \mathbf{m} | 1 - (\hat{H} - E_0)\Delta\tau | \mathbf{n} \rangle$$

is interpreted as the probability of the system of switching the occupation of the state $|\mathbf{n}\rangle$ into the occupation of the state $|\mathbf{m}\rangle$. This propagation has in principle the same properties of the coordinates space version.

Fock space calculations

Unfortunately matrix elements for a many-Fermion systems are not positive definite. It is possible, however, to introduce an importance sampling using a variational ansatz of the wave function to circumvent this problem.
First one redefines the Hamiltonian as:

$$\langle \mathbf{m}|\mathcal{H}_\gamma|\mathbf{n}\rangle = \begin{cases} -\gamma\langle \mathbf{m}|H|\mathbf{n}\rangle & \mathfrak{s}(\mathbf{m},\mathbf{n}) > 0 \\ \langle \mathbf{m}|H|\mathbf{n}\rangle & \text{otherwise} \end{cases}$$

for the off-diagonal terms and

parameter: if > 0, no sign problem, but biased result. Extrapolation to -1 gives the exact result (or at least a rigorous upper bound)

$$\langle \mathbf{n}|\mathcal{H}_\gamma|\mathbf{n}\rangle = \langle \mathbf{n}|H|\mathbf{n}\rangle + (1+\gamma) \sum_{\substack{\mathbf{m}\neq\mathbf{n} \\ \mathfrak{s}(\mathbf{m},\mathbf{n})>0}} \mathfrak{s}(\mathbf{m},\mathbf{n}) \ .$$

for the diagonal terms, with:

$$\mathfrak{s}(\mathbf{m},\mathbf{n}) = \Phi_G(\mathbf{m})\langle \mathbf{m}|H|\mathbf{n}\rangle/\Phi_G(\mathbf{n})$$

Variational function (explicit)

Fock space calculations

We now define a new propagator:

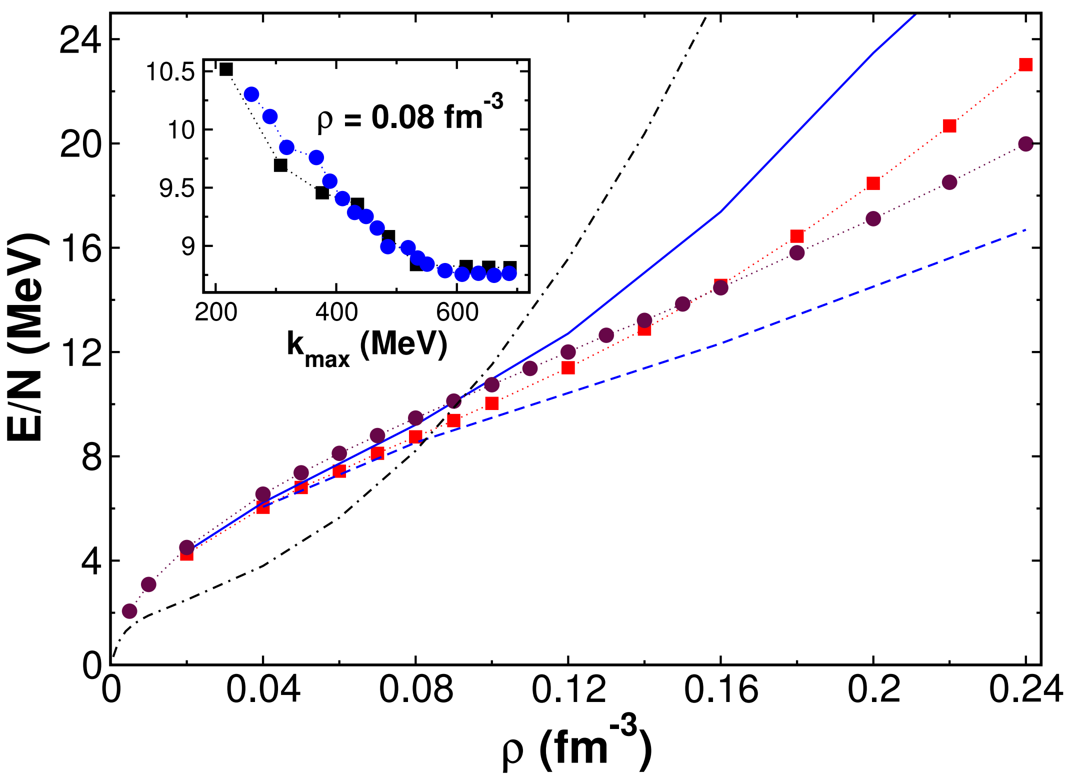
$$\langle \mathbf{m}|\mathcal{P}_\gamma|\mathbf{n}\rangle = 1 - \Delta\tau \Phi_G(\mathbf{m})\langle \mathbf{m}|\mathcal{H}_\gamma - E_T|\mathbf{n}\rangle/\Phi_G(\mathbf{n}) \ .$$

The propagator $\mathcal{P}_\gamma$, by construction, is free from the sign problem for $\gamma \geq 0$, and filters out the wave function $\Phi_G(\mathbf{n})\Psi_\gamma(\mathbf{n})$, where $\Psi_\gamma(\mathbf{n})$ is the ground state wave function of $\mathcal{H}_\gamma$

As previously mentioned, the choice of the representation of the Hilbert space is arbitrary!

- FINITE SYSTEMS ➔ ***H.O. basis, Gaussians, HH..***
- INFINITE SYSTEMS ➔ ***Plane waves, BCS,…***

Configuration Interaction Monte Carlo

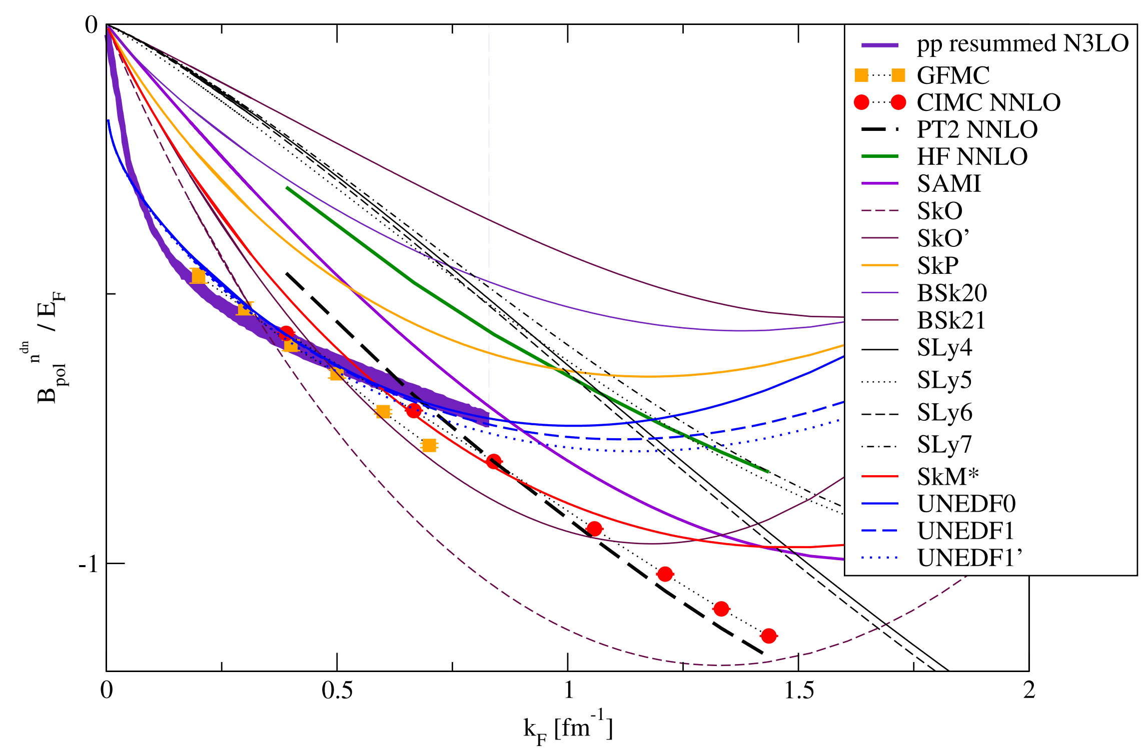


One of the main advantages of using an algorithm in Fock space is the **possibility of using non-local Hamiltonians**, such as the ***chiral EFT based Hamiltonians.***

Here on the left, the computation of the equation of state of pure neutron matter with the 2-body N2LO(opt) interaction of Machleidt et al. and using as importance functions the result of a CC calculation at the SD level.

Alessandro Roggero, Abhishek Mukherjee, Francesco Pederiva
PRL, in press (2014)

On the right the energy of a neutron polaron, always computed with the same Hamiltonian and CIMC.



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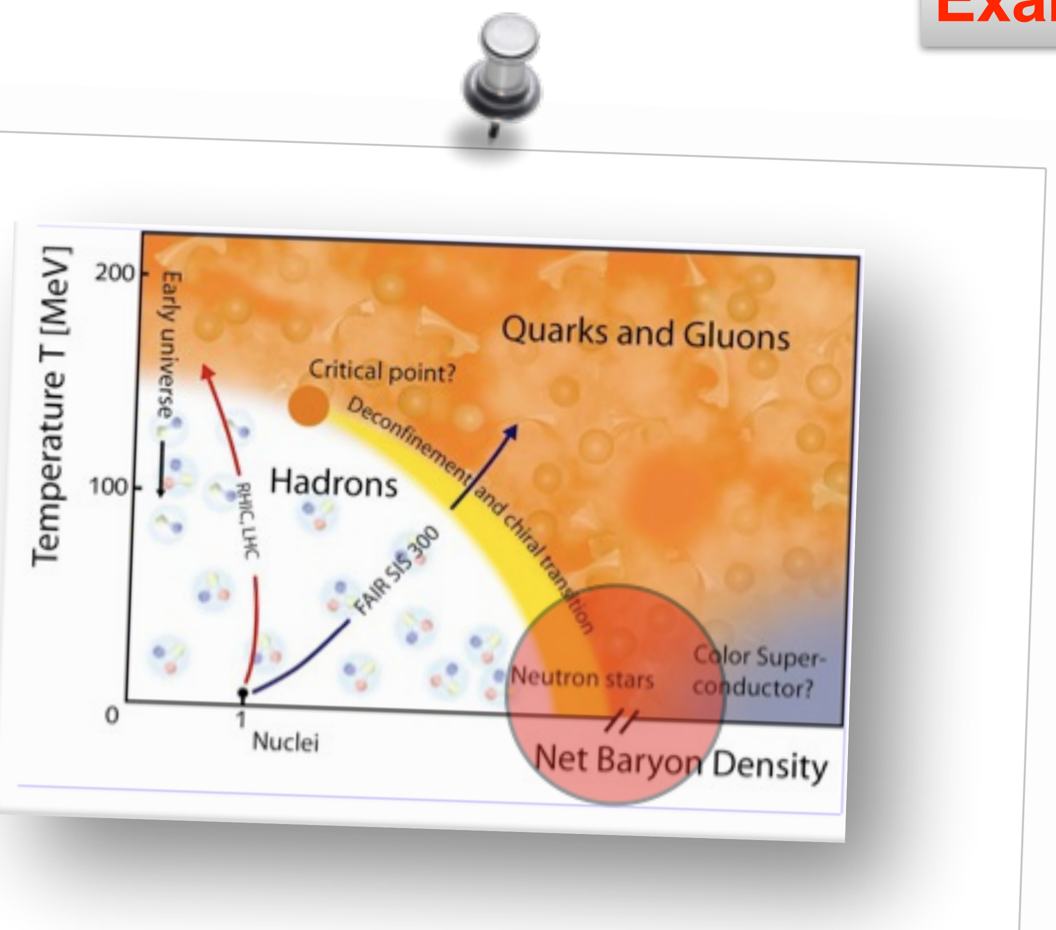
Open questions...

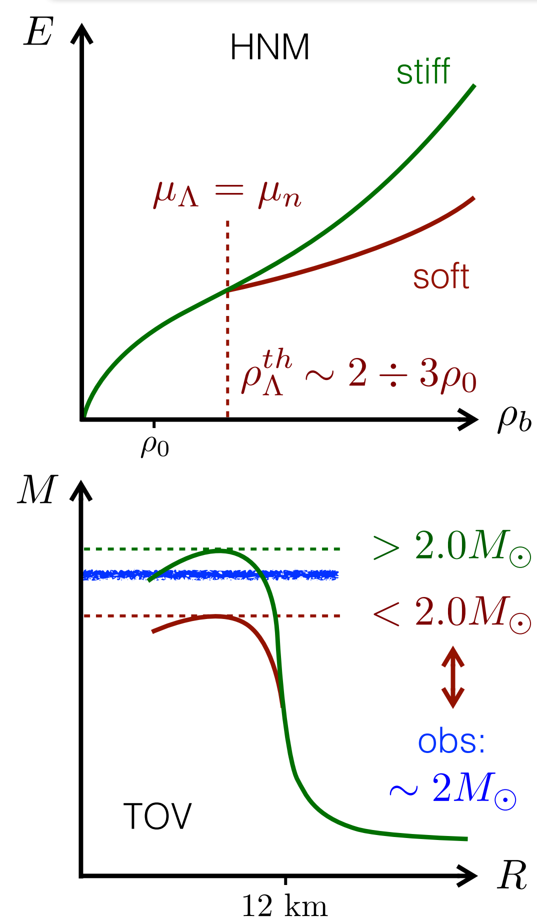
The *fine tuning* of the hyperon-nucleon interaction is essential to understand the behaviour of matter in extreme conditions.

Example: Neutron stars

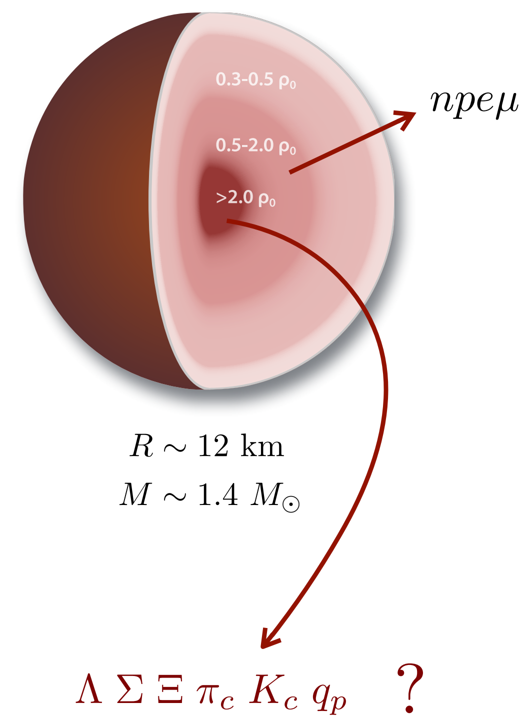


Far away from any possible perturbative treatment..

Equation of state



Neutron star structure

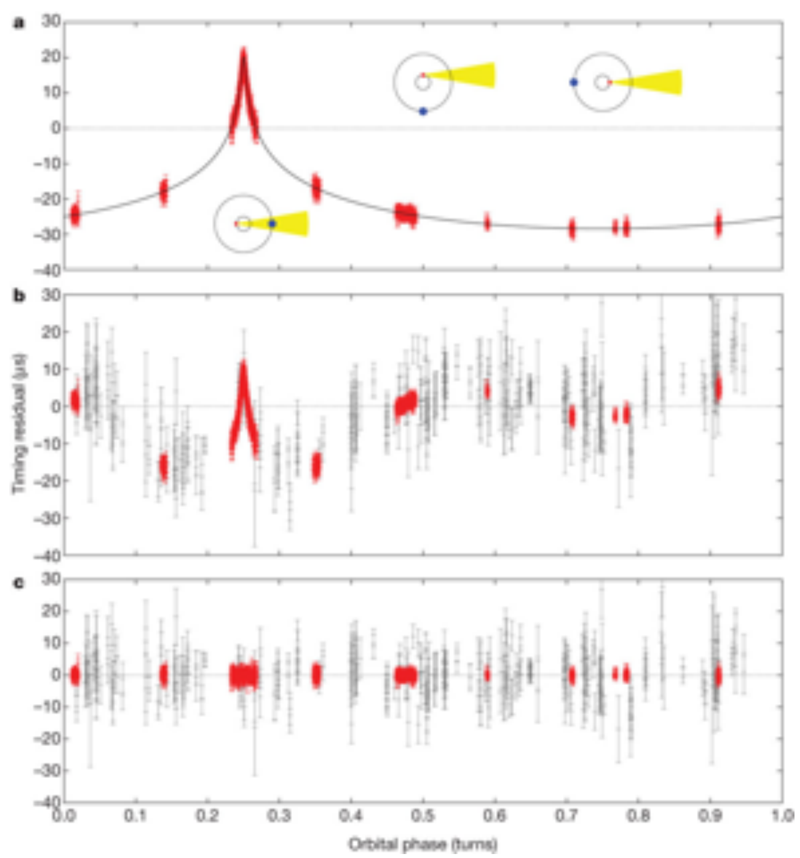


Internal composition still largely unknown

Hyperon Puzzle

A few NS with a large mass were observed by using Shapiro delay measurements. The first (2010) was PSRJ1614-2230 pulsar with **M=1.97(4)M⊙**.

(P. B. Demorest, T. Pennucci, S. M. Ransom, M. S. E. Roberts and J. W. T. Hessels. A two-solar-mass neutron star measured using Shapiro delay measurements, Nature 467, 1081 (2010).



In a non relativistic framework (= pure baryonic stars) hyperons are problematic

Before 2010:

Maximum mass observed: 1.6M⊙

Maximum mass predicted without hyperons: 2.3⊙ (still ok in principle)

Maximum mass predicted with hyperons: 1.4-1.6M⊙ (good!)

After 2010:

Observed mass: 2.0M⊙

Maximum mass predicted without hyperons: 2.3M⊙ (good!)

Maximum mass predicted with hyperons: 1.4-1.6M⊙ (very bad…)

Many possible description of the YN interaction

NON RELATIVISTIC:

write an Hamiltonian including some potential and try to solve a many-body Schroedinger equation.

- The potential energy is not an observable: several different equivalent descriptions are possible.
- The interaction can be based on some more or less phenomenological scheme (fit the existing experimental data, rely on some systematic meson exchange model), or can be inferred from EFT systematic expansions.
- Only accurate many-body calculations can help distinguishing among different realizations of the potential.

RELATIVISTIC:

write a Lagrangian including relevant fields, and try to solve the field theoretical problem (usually RMF calculations are performed).

Some hints from LQCD.....

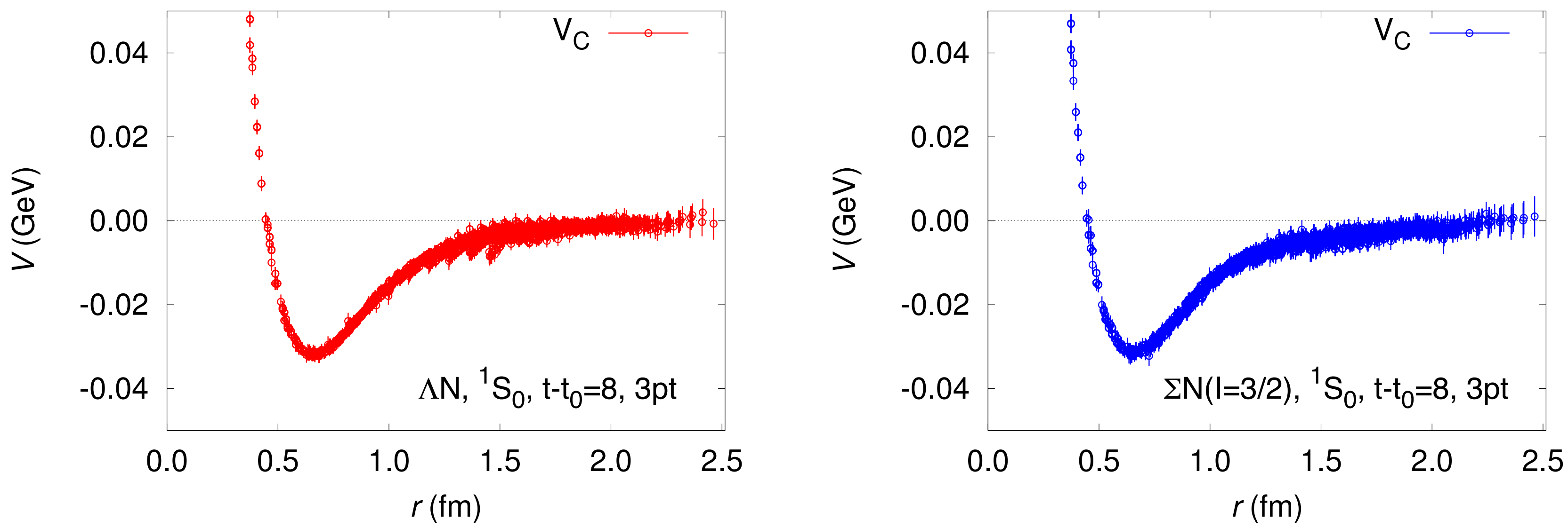


Fig. 10. Left: The central potential in the $^1S_0$ channel of the ΛN system in $2+1$ flavor QCD as a function of r. Right: The central potential in the $^1S_0$ channel of the $\Sigma N(I=3/2)$ system as a function of r.

S. Aoki et al. (HAL-QCD collaboration)

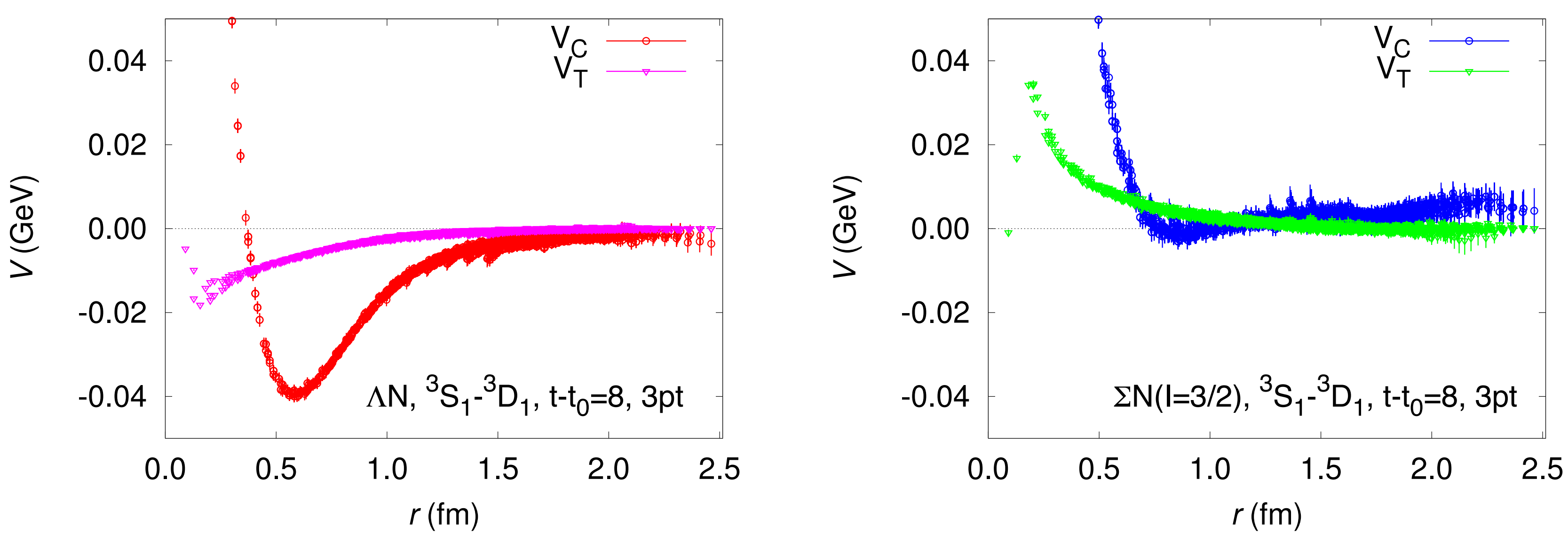
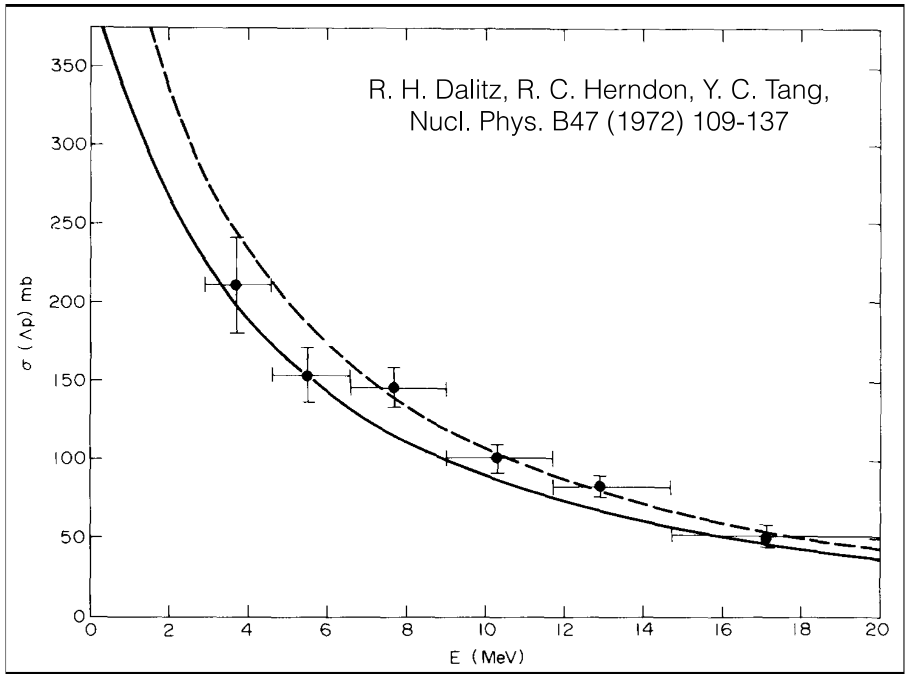


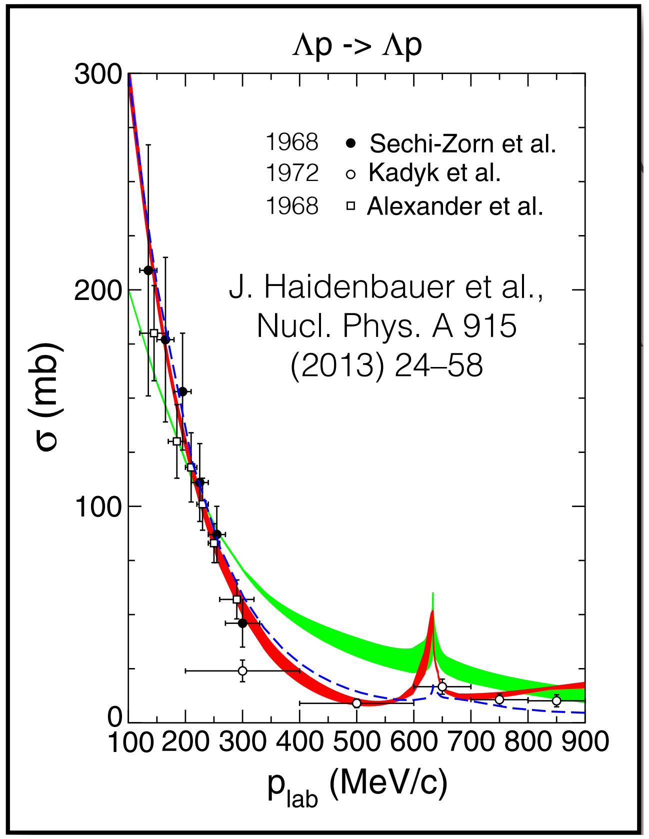
Fig. 11. Left: The central potential (circle) and the tensor potential (triangle) in the $^3S_1 -^3 D_1$ channel of the ΛN system as a function of r. Right: The central potential (circle) and the tensor potential (triangle) in the $^3S_1 -^3 D_1$ channel of the $\Sigma N(I=3/2)$ system as a function of r.

Hard cores seem to be unavoidable in a realistic description!

Model Hyperon-nucleon interaction

In order to gain some understanding, we need to set up some scheme.





OUR CHOICE

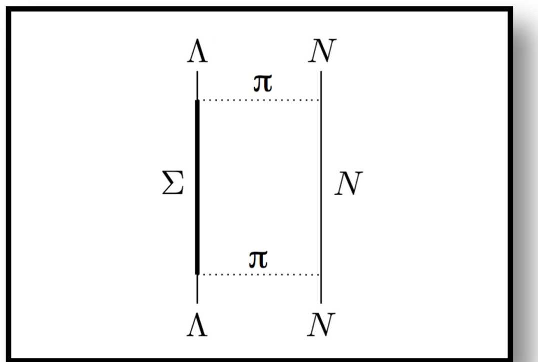
- **NON RELATIVISTIC APPROACH** (should be fine if the central density is not too large)
- **YN INTERACTION CHOSEN TO FIT EXISTING SCATTERING DATA** (with a hard-core)
- **PHENOMENOLOGICAL YNN THREE-BODY FORCES** with few parameters to be adjusted to reproduce light hypernuclei binding energies
- **ALL THE OTHER RESULTS ARE PREDICTIONS WITH NO OTHER ADJUSTABLE PARAMETERS** obtained from an *accurate solution of the Schroedinger equation*.

- **THIS IS ONE OF MANY POSSIBLE WAY TO ATTACK THE PROBLEM.**
- **EMPHASIS IS ON EXPERIMENTALLY AVAILABLE INFORMATION.**

Model Hyperon-nucleon interaction

Model interaction (Bodmer, Usmani, Carlson):

A. Bodmer, Q. N. Usmani, and J. Carlson, Phys. Rev. C 29, 684 (1984).

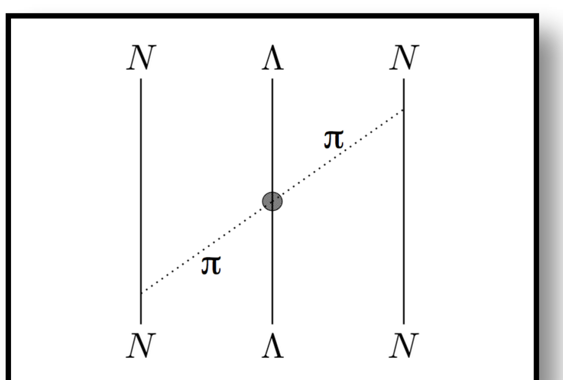


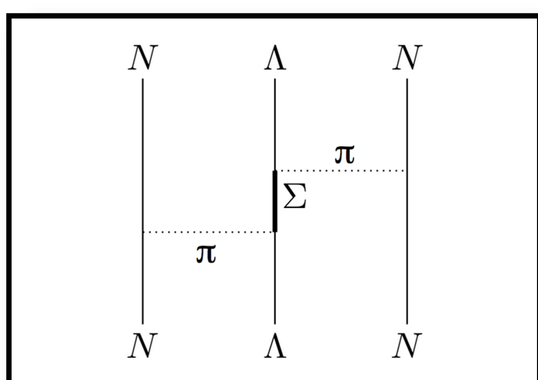
from Kaon exchange terms (not considered explicitly in our calculations)

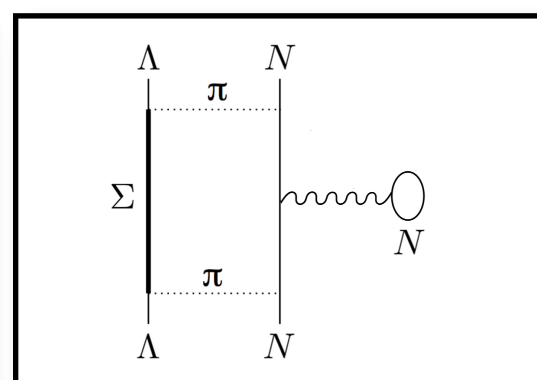
$$V_{\Lambda i}(r) = v_0(r) + v_0(r)\varepsilon(P_x - 1) + \frac{1}{4}v_\sigma T_\pi^2(m_\pi r)\boldsymbol{\sigma}_\Lambda \cdot \boldsymbol{\sigma}_i$$

Two-body potential: accurately fitted on p-*Λ* scattering data

Q. N. Usmani and A. R. Bodmer, Phys. Rev. C 60, 055215 (1999).







$$V_{\Lambda ij} = V_{\Lambda ij}^{2\pi} + V_{\Lambda ij}^{D}$$

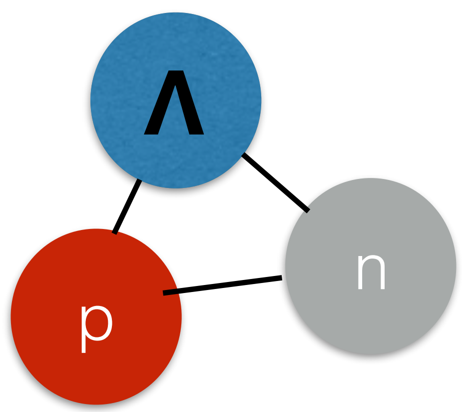
$$\begin{cases} V_{\Lambda ij}^{2\pi} = C_{2\pi}^{SW}\mathcal{O}_{\Lambda ij}^{2\pi,SW} + C_{2\pi}^{PW}\mathcal{O}_{\Lambda ij}^{2\pi,PW} \\ V_{\Lambda ij}^{D} = W^D\, T_\pi^2(m_\pi r_{\Lambda i})\, T_\pi^2(m_\pi r_{\Lambda j}) \left[1 + \frac{1}{6}\boldsymbol{\sigma}_\Lambda \cdot (\boldsymbol{\sigma}_i + \boldsymbol{\sigma}_j)\right] \end{cases}$$

Parameters to be determined from calculations

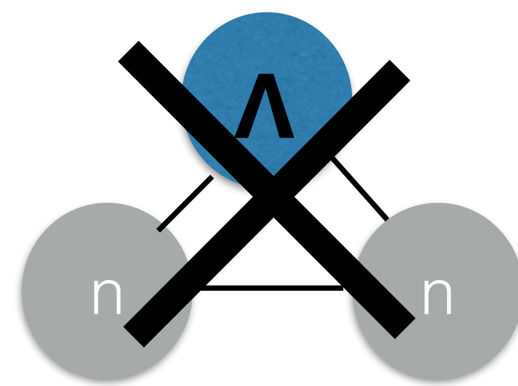
Non trivial isospin dependence in the three-body sector?

In hypernuclei it is possible that the ΛNN interaction is not well constrained, especially in the isospin triplet channel:

NN isospin singlet



NN isospin triplet



Pauli repulsion

On can try o do the exercise of re-projecting the interaction in the isospin singlet and triplet channels and try to explore the dependence of the hypernuclei binding energy on the relative strength.

must be **negative on average** to give repulsion

C_T=1 gives the original potential, but we can choose an **arbitrary value**.
$C_T < 1 \Rightarrow$ more repulsion

$$v^{2\pi,P} = -\frac{C_P}{6}\left\{X_{i\lambda}, X_{\lambda j}\right\}\vec{\tau}_i\cdot\vec{\tau}_j$$

$$v^{2\pi,S} = C_S O^{2\pi,S}_{ij\lambda}\vec{\tau}_i\cdot\vec{\tau}_j$$

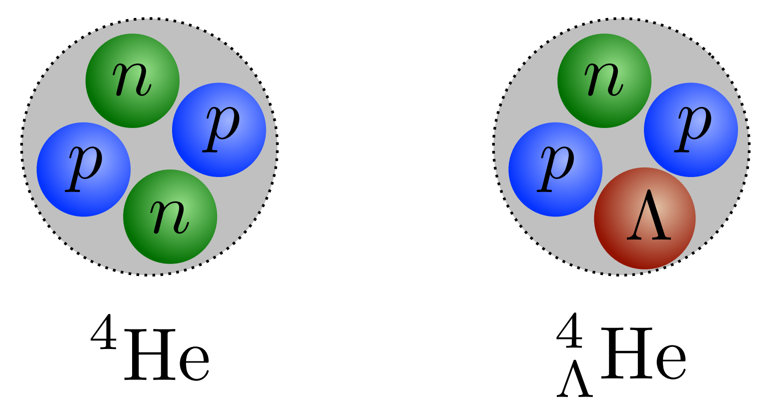
$$v^{\tau\tau}_{ij\lambda} = -3v^{P}_{ij\lambda}\hat{P}^{T=0}_{ij} + C_T v^{P}_{ij\lambda}\hat{P}^{T=1}_{ij}$$

$$v^{\tau\tau}_{ij\lambda} = \frac{3}{4}(C_T-1)v^{P}_{ij\lambda} + \frac{1}{4}(3+C_T)v^{P}_{ij\lambda}\vec{\tau}_i\cdot\vec{\tau}_j$$

Input from experiment

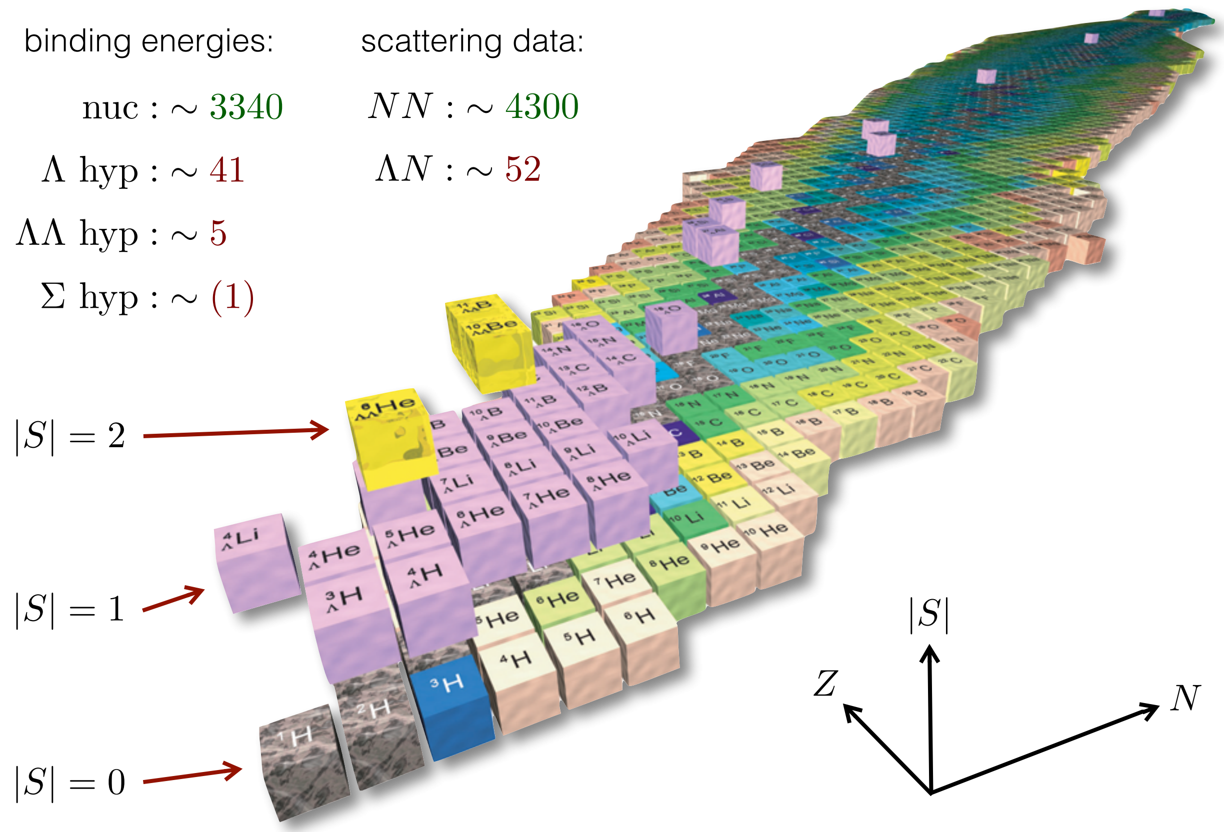
We need to fit the three body interaction against some experimental data. There are available several measurements of the binding energy of *Λ*-hypernuclei, i.e. nuclei containing a Λ hyperon. The idea is to compute such binding energies. We can then compute the **hyperon separation energy:**

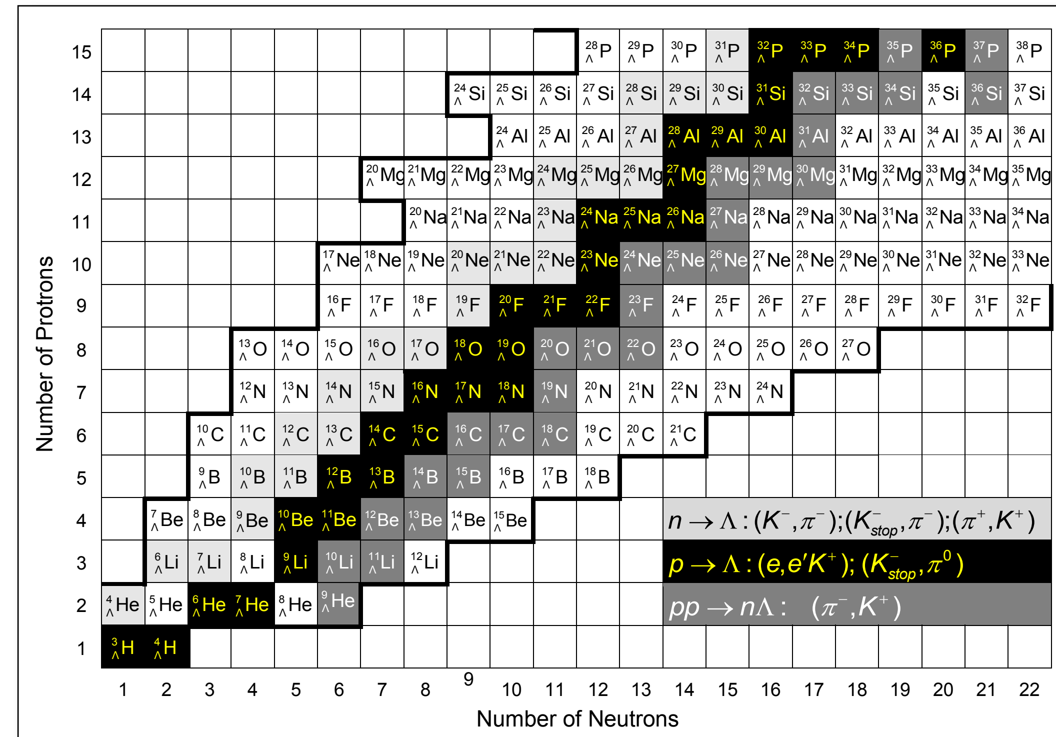
$$B_\Lambda = B_{hyp} - B_{nuc}$$



where B_{hyp} is the total binding energy of a hypernucleus with A nucleons and one Λ , and B_{nuc} is the total binding energy of the corresponding nucleus with A nucleons. This number can be used to gauge the coefficients in the nucleon-Λ interaction.

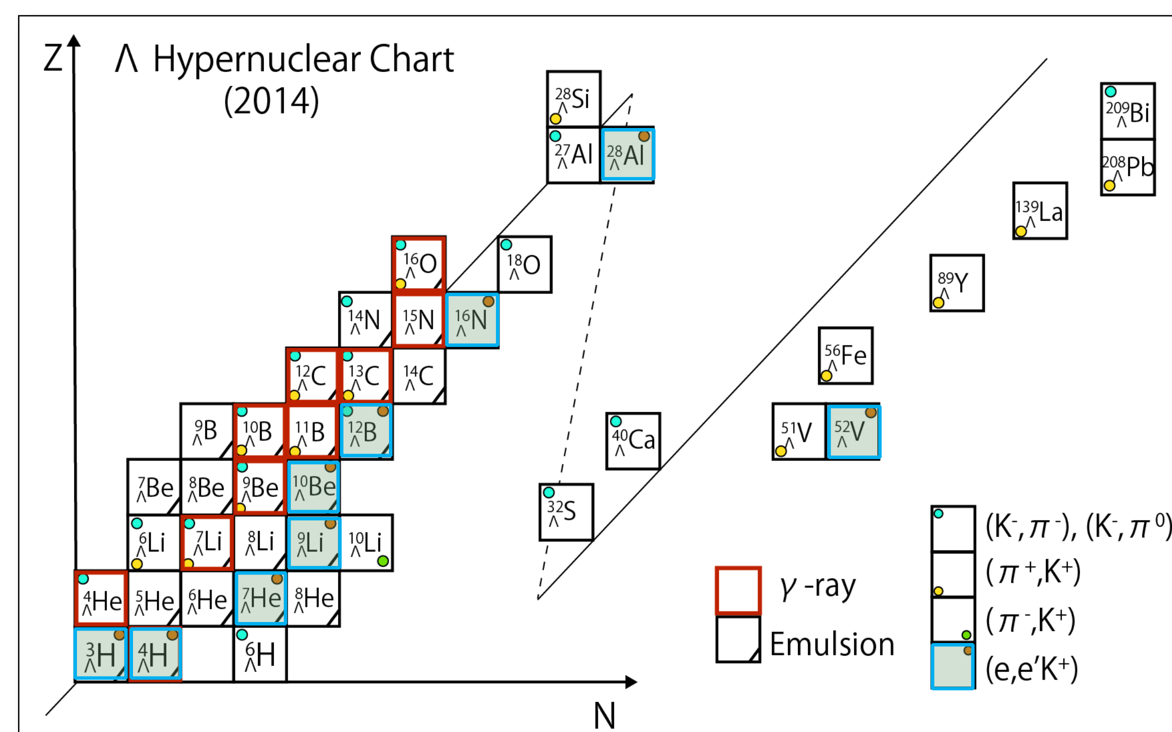
Hypernuclei data





J. Pochodzalla, Acta Phys. Polon. B 42, 833– 842 (2011)

- The available data are very limited.
- There are several planned and ongoing systematic measurements.
- At present no proposals for gathering more Λ-nucleon scattering data
- Essentially no information on $\Lambda\Lambda$ interaction
- (Almost) nothing on Σ or Ξ hypernulcei



S. N. Nakamura, Hypernuclear workshop, JLab, May 2014
updated from: O. Hashimoto, H. Tamura, Prog. Part. Nucl. Phys. 57, 564 (2006)

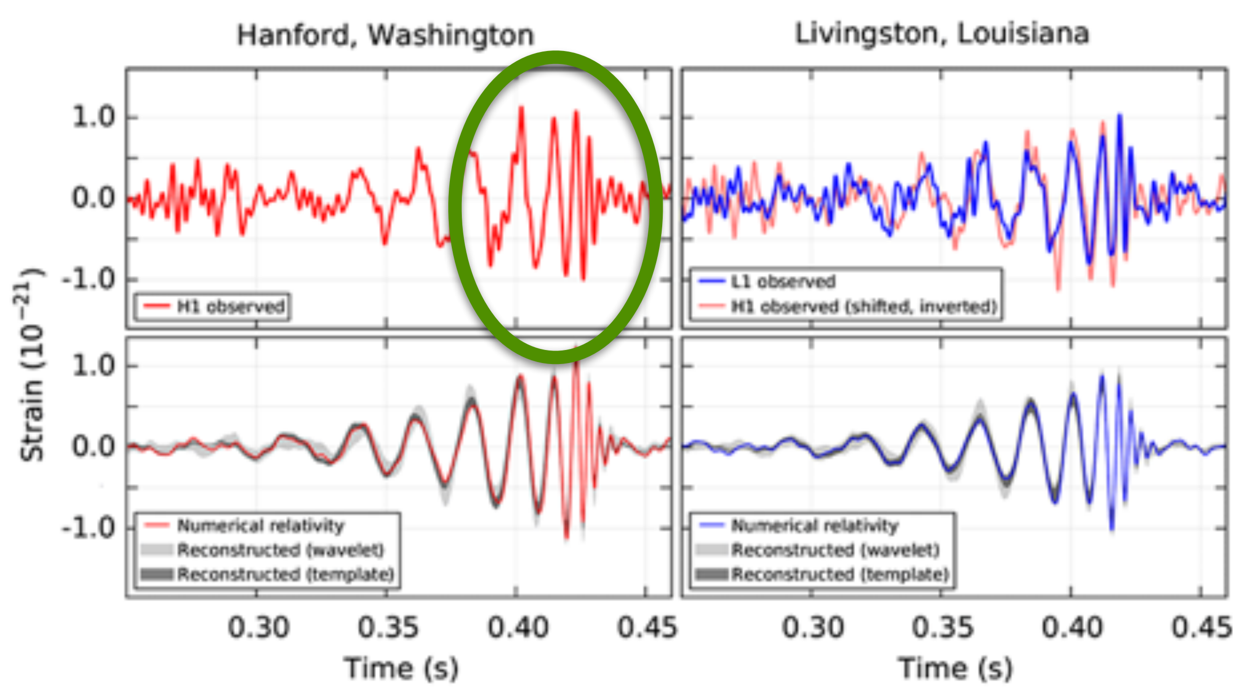
Gravitational waves

The EoS of dense matter is one of the ingredients needed in the **solution of Einstein's** equation when studying the dynamics of **neutron star mergers.**

How sensitive is the spectrum of GW on the details of the EoS?

There is a region within a few ms away from the actually merging where the spectrum seems to become rather sensitive on the stiffness, at the post that the GW spectrum might be used in this case to determine the NS radius with an accuracy of about 1Km.

If such events will be experimentally observed, a completely **new kind of constraints** will be provided. Will we be ready for that?



These were two BHs. Too bad…

Warning: temperature, neutrinos…

Gravitational waves

PRL 115, 091101 (2015) PHYSICAL REVIEW LETTERS week ending 28 AUGUST 2015

Modeling the Complete Gravitational Wave Spectrum of Neutron Star Mergers

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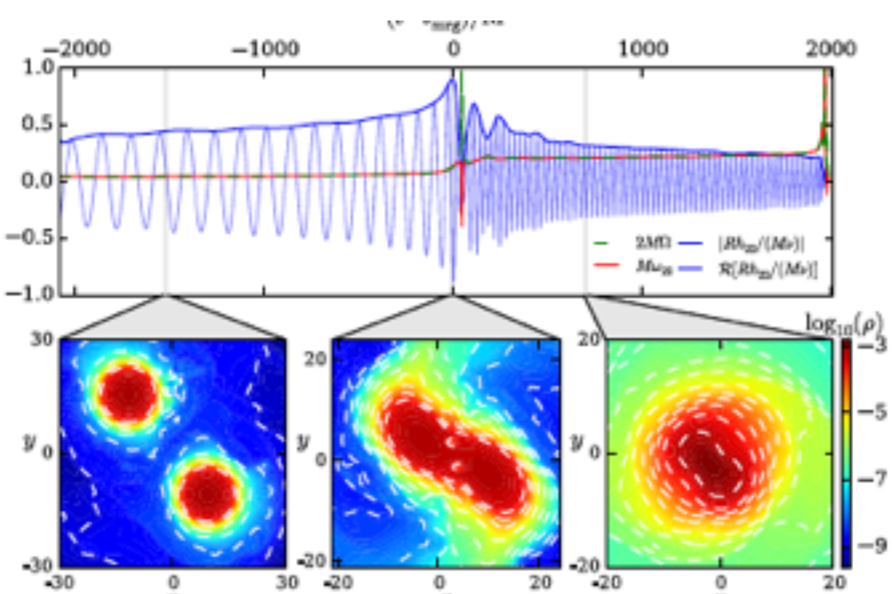
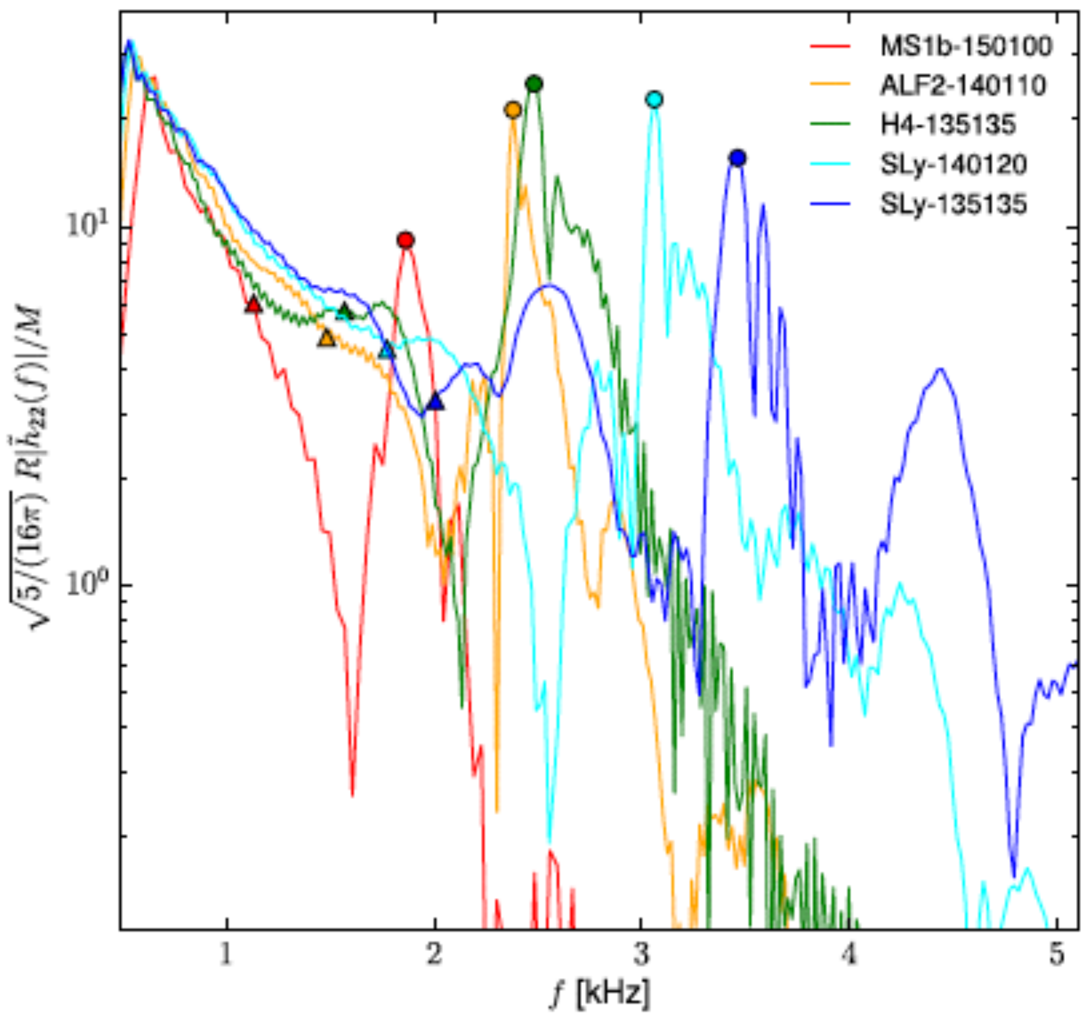
(Received 9 April 2015; revised manuscript received 11 June 2015; published 27 August 2015)

Introduction.—Direct gravitational wave (GW) observations of binary neutron stars (BNS), late-inspiral merger and postmerger by ground-based GW interferometric experiments, can lead to the strongest constraints on the equation of state (EOS) of matter at supranuclear densities [1–7]. There are two ways to set such constraints (GW observations of BNS mergers can also constrain the source redshift [8,9]): (I) measure the binary phase during the last minutes of coalescence using matched filtered searches [1,3–5] and (II) measure the postmerger GW spectrum frequencies using burst searches [6,7].





Different EoS fitted with polytropic functions…

Conclusions

- AFDMC calculations are evolving. Better accuracy, better performance. This reflects on the work on hypernuclei (see Diego Lonardoni's talk).
- Accessible systems: definitely A=90. For heavier systems one can possibly use alternative approaches.
- Our philosophy in attacking the problem of the hyperon-nucleon interaction: **we do not want to add more information than the one that the experiments can give us.** Having too many parameters will result in a substantially **arbitrary prediction of the EoS**, and consequently **adjustable predictions on the Neutron Star structures**.

SUPPLEMENTAL MATERIAL

Projection Monte Carlo

We should also write the propagator in coordinates space, so that:

$$\langle R|\Psi(\tau)\rangle = \langle R|e^{-(\hat{H}-E_0)\tau}|R'\rangle\langle R'|\Psi(0)\rangle$$

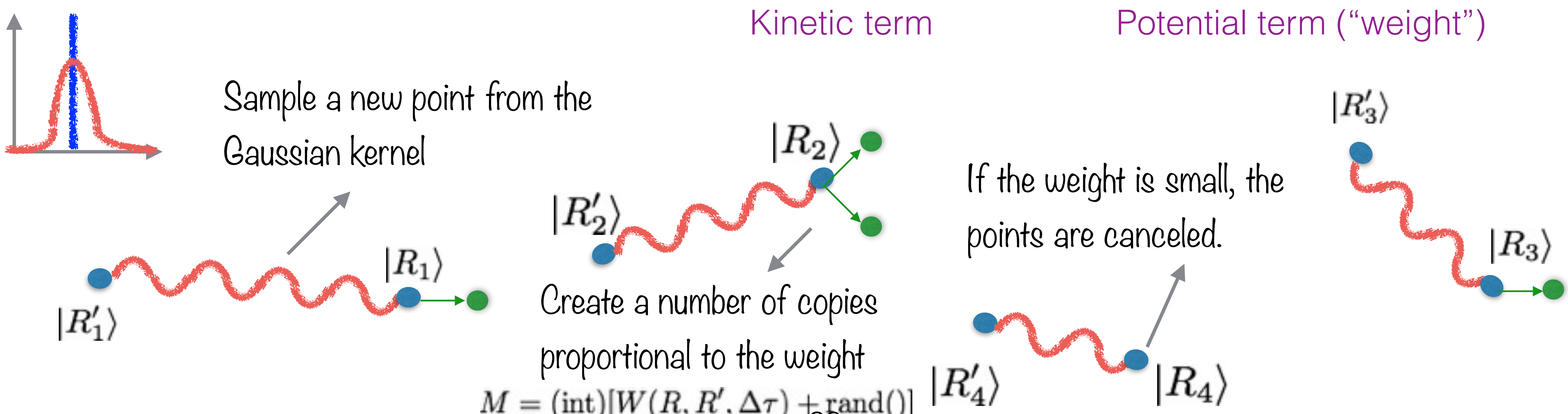
In the limit of "short" τ (let us call it "$\boldsymbol{\Delta\tau}$"), the propagator can be broken up as follows (Trotter-Suzuki formula):

$W(R, R', \Delta\tau)$

$$\langle R|e^{-(\hat{H}-E_0)\Delta\tau}|R'\rangle \sim e^{-\frac{(R-R')^2}{2\frac{\hbar}{m}\Delta\tau}}\, e^{-\left(\frac{V(R)+V(R')}{2}-E_0\right)\Delta\tau}$$

Kinetic term

Potential term ("weight")



Projection Monte Carlo

Once the convergence to the ground state is reached it is possible to use the sampled configurations to evaluate expectations of observables of interest in a Monte Carlo way. For example, if we want to compute the energy, we can use some test function and evaluate the following ratio:

$$\frac{\sum_k \hat{H}\Psi_T(R_k)}{\sum_k \Psi_T(R_k)}$$

This is the Monte Carlo estimate of:

$$\frac{\int dR \Psi_0(R)\hat{H}\Psi_T(R)}{\int dR \Psi_0(R)\Psi_T(R)} = \frac{\langle\Psi_0|\hat{H}|\Psi_T\rangle}{\langle\Psi_0|\Psi_T\rangle} = \frac{\langle\Psi_T|\hat{H}|\Psi_0\rangle}{\langle\Psi_T|\Psi_0\rangle} = E_0$$

Known issues

- **The naive algorithm does not work for any realistic potential. In general the random walk needs to be guided by an "importance function". In a correct formulation there is no bias on the results.**

- **The algorithm works (strictly speaking) only for the "mathematical" ground state of the Hamiltonian, which is always a symmetric (bosonic) wavefunction. Fermions live on an "mathematical excited state" of H! ➡ SIGN PROBLEM. Workarounds exist, but the results are biased. However, in some cases it is possible to estimate the bias.**

Many-nucleon systems

Nuclear physics experiments teach us that the nucleon-nucleon interaction depends on the relative spin and isospin state of nucleons. This fact can be formally related to the fundamental symmetry properties of QCD, and it is necessary in any realistic interactions that can be used in a many-body calculation

EXAMPLE: One of the most celebrated model nucleon-nucleon (NN) interaction is the so-called Argonne AVX potential, defined by:

$$\langle R, S, T | V_X \rangle = \sum_{i=1}^{X} v_i(r_{ij}) \hat{O}^i$$

R B Wiringa, V G J Stoks, and R Schiavilla PRC 51, 38 (1995)

Spin representation in term of Pauli matrices

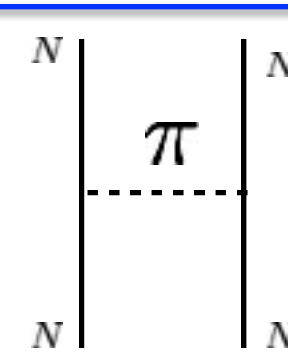
Spin-orbit

Isospin

EX: AV8

$$\{\mathbb{I}, \vec{\sigma}_i \cdot \vec{\sigma}_j, S_{ij}, \hat{L}_{ij} \cdot \frac{1}{2}(\vec{\sigma}_i + \vec{\sigma}_j)\} \otimes \{\mathbb{I}, \vec{\tau}_i \cdot \vec{\tau}_j\}$$

Here S_{ij} is the tensor operator



$$S_{ij} \equiv 3(\hat{r}_{ij} \cdot \vec{\sigma}_i)(\hat{r}_{ij} \cdot \vec{\sigma}_{ij}) - \vec{\sigma}_i \cdot \vec{\sigma}_j$$

that characterises the “one-pion exchange” part of the interaction.

Projection MC many-nucleon systems

We can apply our (very general) propagator to a state that is now given by the particle positions (the "R"), and the spin/isospin state of each nucleon (the "S").

Problem

In the stochastic evolution, spins are subject to factors like:

$$\langle R, S| e^{-\sum_{ij} v_{\sigma\sigma}(r_{ij}) \vec{\sigma}_i \cdot \vec{\sigma}_j \Delta\tau} |R, S'\rangle$$

But:

$$\vec{\sigma_i} \cdot \vec{\sigma_j} |S\rangle = \begin{cases} -3/4|S\rangle & \text{if } i,j \text{ in } S=0 \text{ state} \\ 1/4|S\rangle & \text{if } i,j \text{ in } S=1 \text{ state} \end{cases}$$

The action of the propagators depends on the relative spin state of each pair of nucleons

Projection MC many-nucleon systems

Multicomponent wave functions are needed!
How large is the system space? For a system of A nucleons, Z protons, the number of states is $2^A \binom{A}{Z}$

	A	Pairs	Spin $\times$ Isospin
^{4}He	4	6	8×2
^{6}Li	6	15	32×5
^{7}Li	7	21	128×14
^{8}Be	8	28	128×14
^{9}Be	9	36	512×42
^{10}Be	10	45	512×90
^{11}B	11	55	2048×132
^{12}C	12	66	2048×132
^{16}O	16	120	32768×1430
^{40}Ca	40	780	$3.6 \times 10^{21} \times 6.6 \times 10^9$
^{8}n	8	28	128×1
^{14}n	14	91	8192×1

Number of states in many nucleon wave functions for a few selected nuclei

- Very accurate results, possibility of using accurate wave functions for the evaluation of general estimators (e.g. response functions
- Due to the high computational cost, application limited so far to $A \leq 12$: **COMPUTATIONAL CHALLENGE!**

AFDMC

The operator dependence in the exponent has become linear.

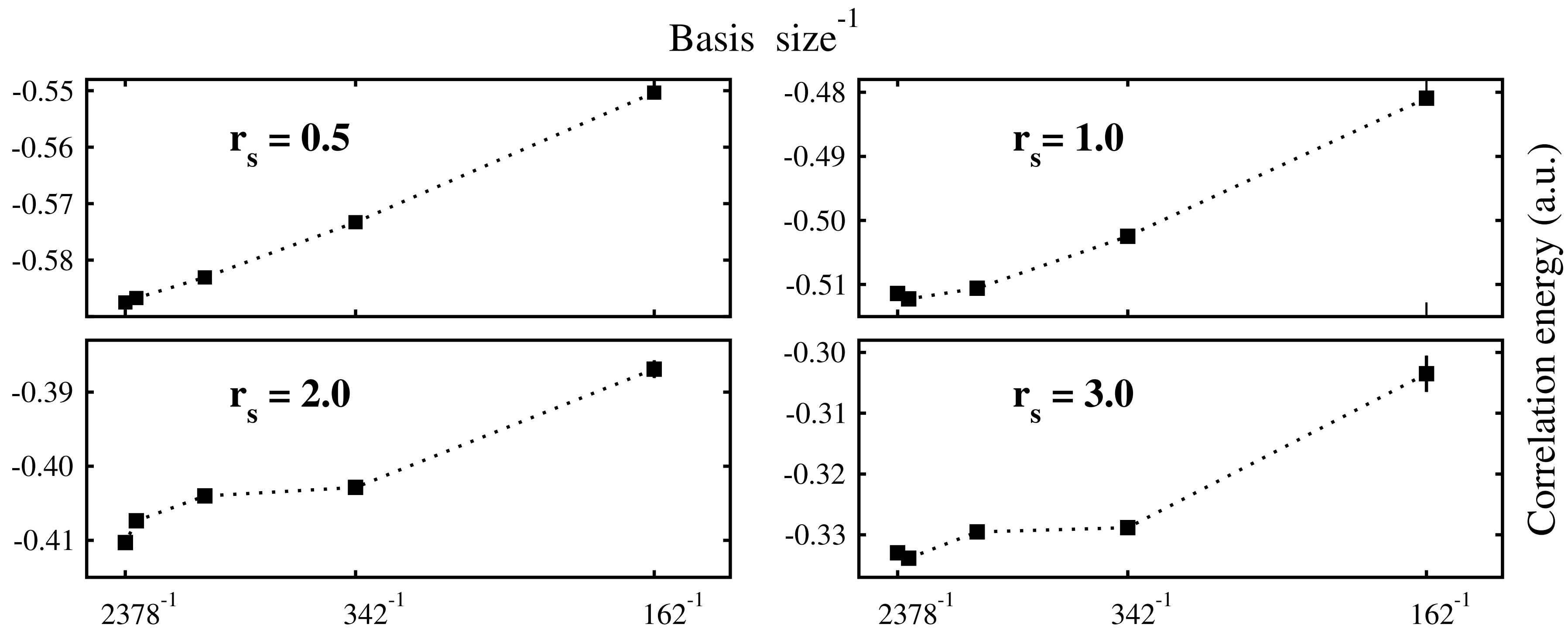
In the Monte Carlo spirit, the integral can be performed by sampling values of x from the Gaussian $e^{-\frac{x^2}{2}}$. For a given *x* the action of the propagator will become:

$$e^{-x\sqrt{\lambda\Delta\tau}\hat{O}_n}|S\rangle = \prod_{k=1}^{3A} e^{-x\sqrt{\lambda\Delta\tau}\phi_n^k\sigma_k}|S\rangle$$

In a space of spinors, each factor corresponds to a rotation induced by the action of the Pauli matrices

The sum over the states
has been replaced by sampling rotations!

Configuration Interaction Monte Carlo



Alessandro Roggero, Abhishek Mukherjee, and Francesco PederivaPhys. Rev. B **88**, 115138 (2013)

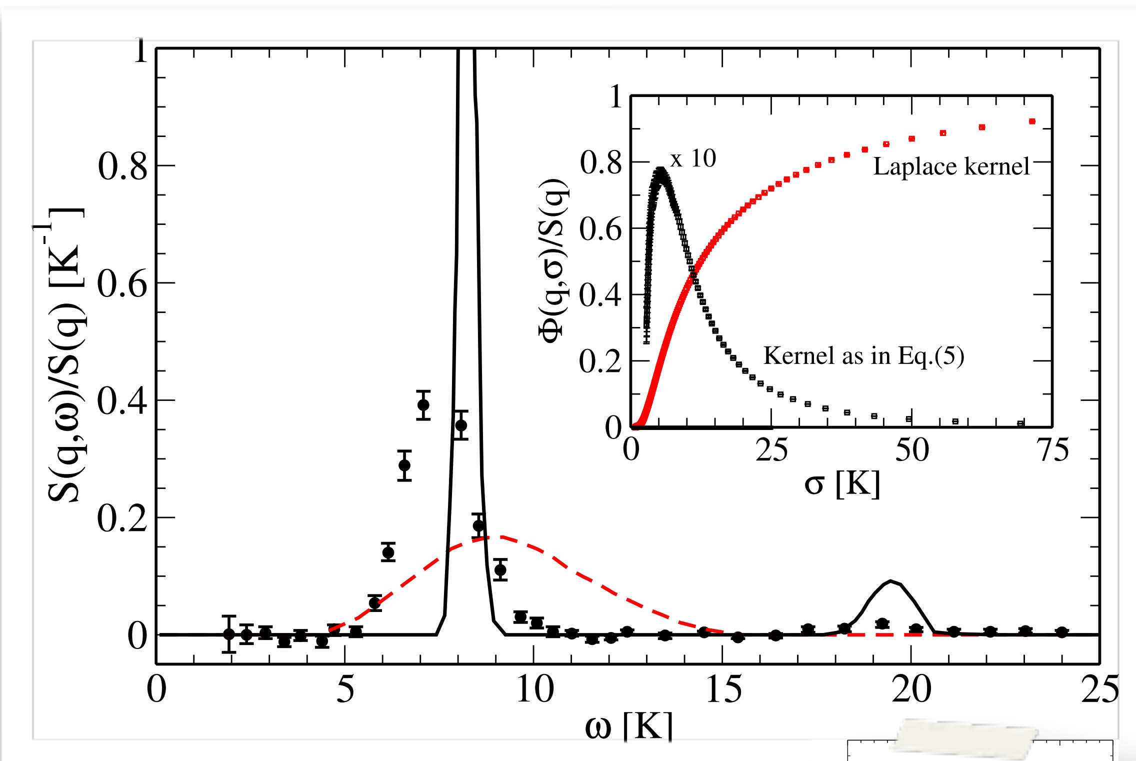
A first test of this algorithm was the evaluation of the equation of state of the three-dimensional homogeneous electron gas, for which very accurate results are already available. In this case the Hamiltonian is very simple, and includes the contribution of a uniform cancelling background of positive charge.

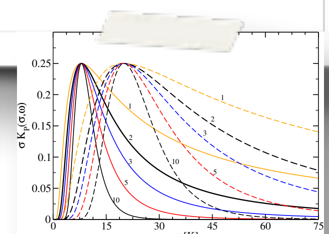
As importance function we used the overlaps computed by COUPLED CLUSTERS at the doubles level (CCD) method.

Response Functions

From QMC calculations

Alessandro Roggero, Francesco Pederiva, and Giuseppina Orlandini, Phys. Rev. B **88**, 094302 (2013)





$$S_{\hat{O}}(\mathbf{q},\omega) = \sum_{\nu} |\langle \Psi_\nu | \hat{O}(\mathbf{q}) | \Psi_0 \rangle|^2 \delta(E_\nu - \omega)$$

$$= \langle \Psi_0 | \hat{O}^\dagger(\mathbf{q}) \delta(\hat{H} - \omega) \hat{O}(\mathbf{q}) | \Psi_0 \rangle$$

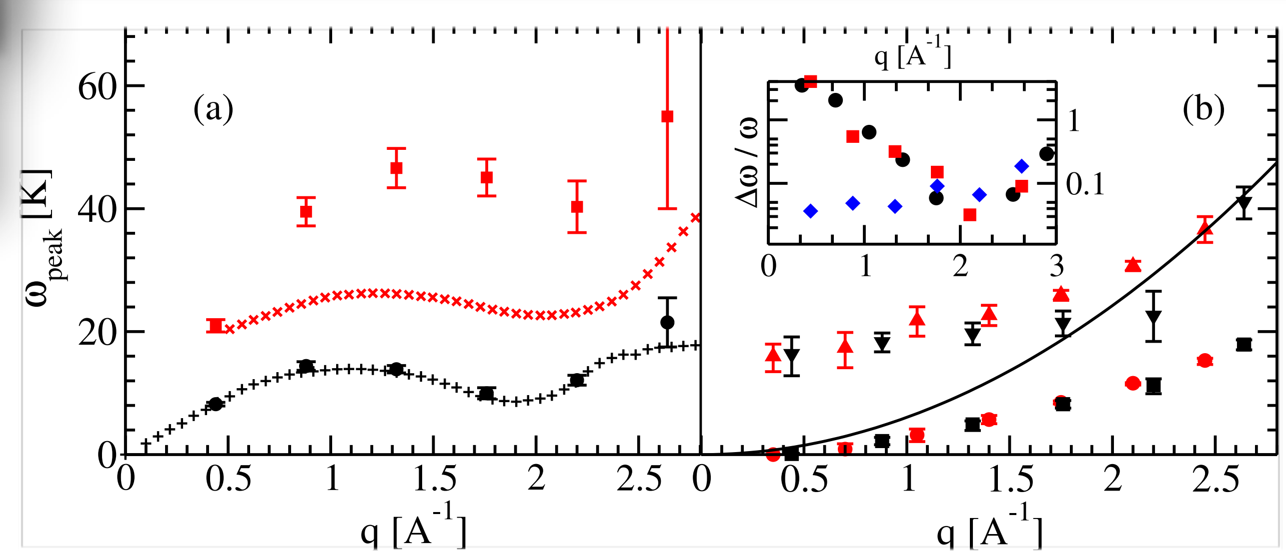
$$\Phi(\mathbf{q},\sigma) = \int K(\sigma,\omega)\, S_{\hat{O}}(\mathbf{q},\omega)\, d\omega.$$

The natural choice within QMC is a Laplace kernel, very inefficient and amplifying the ill-posedness of the inversion problem.

Better kernel: SUMUDU

$$K_P(\sigma,\omega) = N \left[\frac{e^{-\mu \frac{\omega}{\sigma}}}{\sigma} - \frac{e^{-\nu \frac{\omega}{\sigma}}}{\sigma} \right]^P$$

- Still "natural" in the language of QMC
- "Bell shaped", and therefore more efficient and less prone to inversion ambiguities.



Sign Problem

One of the major issues in Quantum Monte Carlo calculations comes from the fact that Fermions live in an excited state (in mathematical sense) of the Hamiltonian. This means that if we want to preserve the normalisation of the Fermionic ground state (using for instance E_0^A instead of E_0 the propagation:

$$e^{-(\hat{H}-E_0^A)\tau}|\Psi\rangle = \sum_{n=0}^{\infty} c_n e^{-(E_n-E_0^A)\tau}|\Psi_n\rangle$$

leads to

Symmetric (bosonic) ground state

Antisymmetric (fermionic) ground state

$$\lim_{\tau\to\infty} e^{-(\hat{H}-E_0^A)\tau} = c_0 e^{-(E_0-E_0^A)\tau}|\Psi_0\rangle + c_0^A|\Psi_0^A\rangle$$

Always > 0 (it's a theorem!)

therefore quantities that are symmetric (like the variance of any operator…) will grow exponentially in imaginary time compared to the expectation of any antisymmetric function. This is the essence of the so called the "sign problem".

Sign Problem

In order to cope with the sign problem it is useful to introduce some approximations. In particular, the general idea is to solve a modified Schroedinger equation with additional boundary conditions.

- For real-valued wave functions, the nodes (zeros) of the solutions must correspond to the nodes of some trial wavefunctions
- **(FIXED NODE APPROXIMATION)**
- For complex valued wave functions, we have two options:
  A. Constrain the phase of the solution to be equal to the phase of some trial wave function **(FIXED PHASE APPROXIMATION)**
  B. Constrain the sign of the real part of the wave function (or some suitable combination) to preserve the sign **(CONSTRAINED PATH APPROXIMATION)**

Thanks!

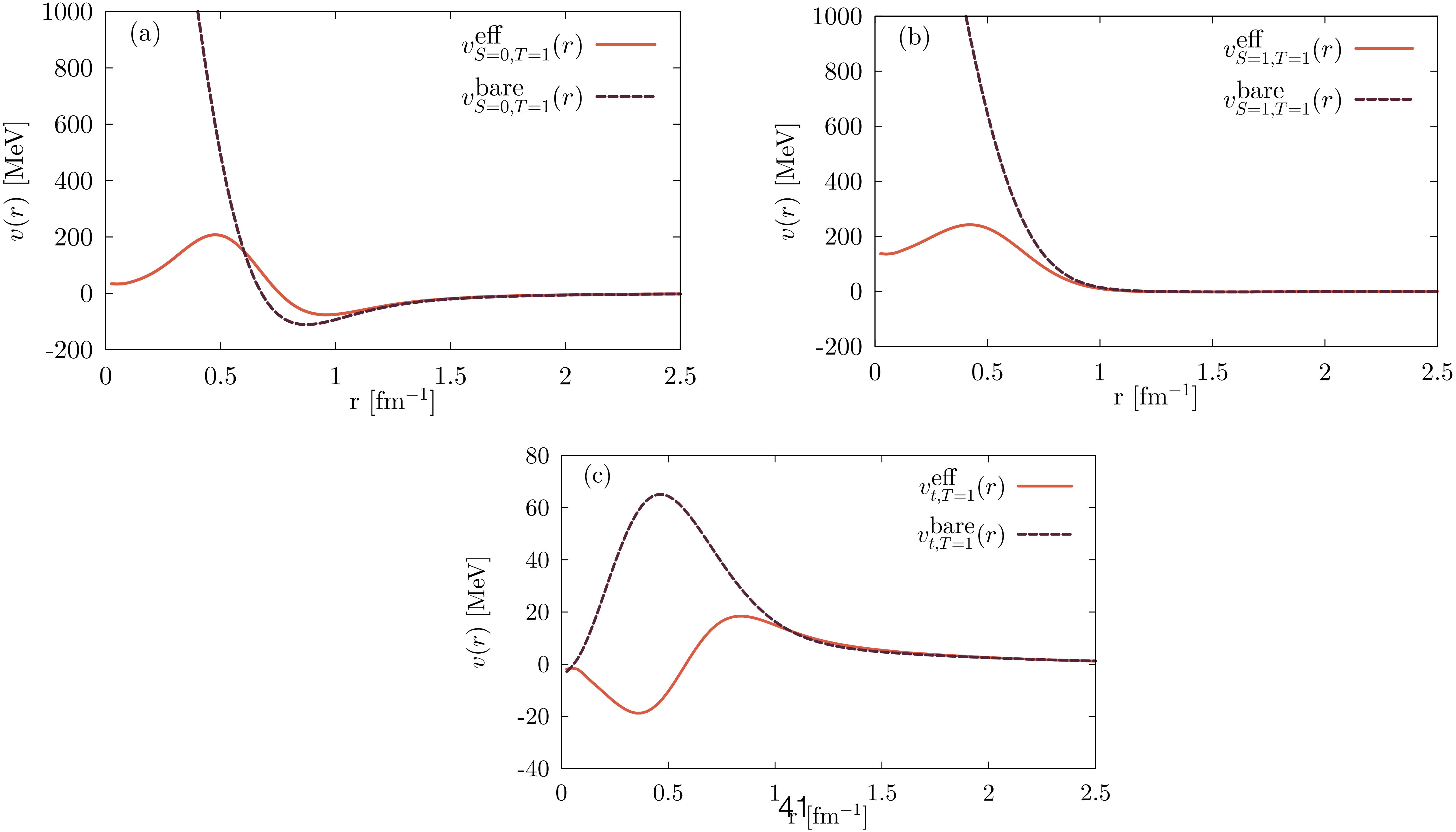
- Stefano Fantoni
- Malvin H. Kalos (LLNL)
- Kevin E. Schmidt (ASU)

- Computer time: NERSC, LLNL, CINECA, ECT*

- Alberto Ambrosetti (MPI-Potsdam)
- Paolo Armani (Trento)
- Omar Benhar (Roma I)
- Francesco Catalano (Trento)
- Lorenzo Contessi (Trento)
- Stefano Gandolfi (LANL)
- Alexey Yu. Illarionov (ETH)
- Diego Lonardoni (ANL)
- Alessandro Lovato (ANL)
- Abhishek Mukherjee (ECT*)
- Giuseppina Orlandini (Trento)
- Alessandro Roggero (Trento)

Effective Interactions

In many cases it is possible to derive effective interactions obtained from the matrix elements of realistic Hamiltonians, computed using advanced many-body approaches.

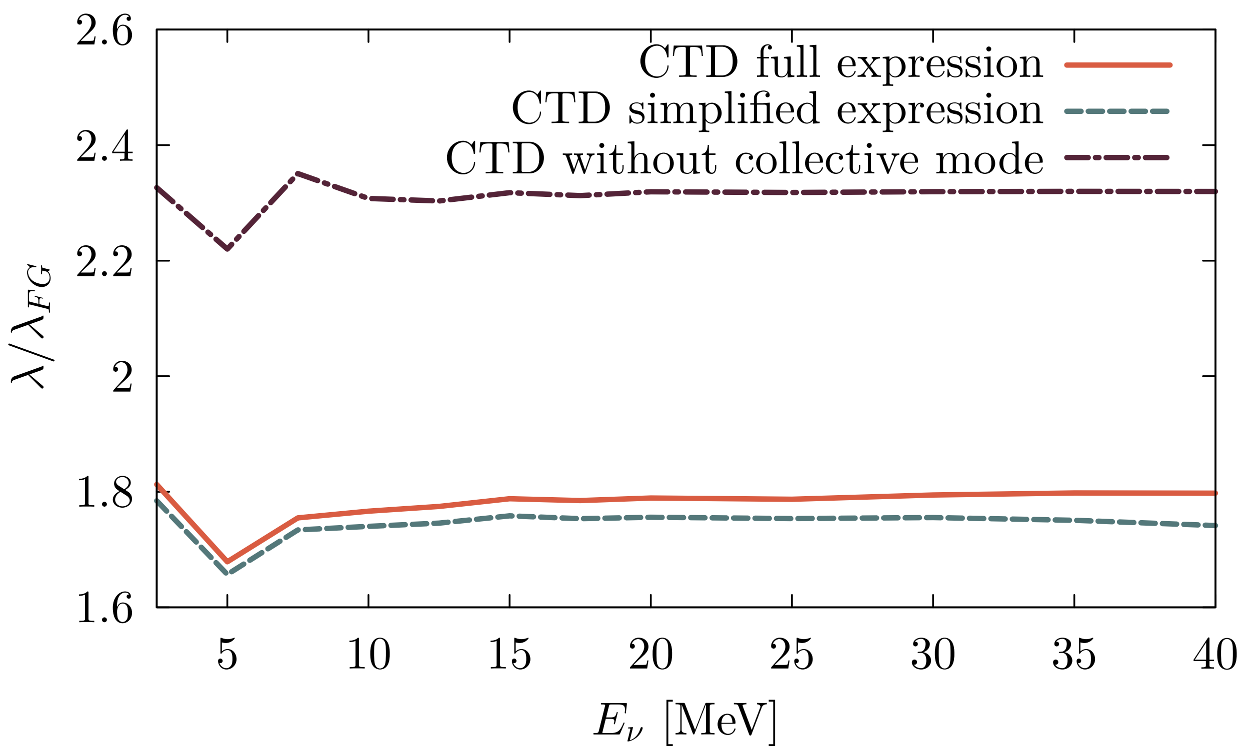


Neutrino mean free path in neutron matter

The mean free path of non degenerate neutrinos at zero temperature is obtained from:

$$\frac{1}{\lambda} = \frac{G_F^2}{4}\rho \int \frac{d^3q}{(2\pi)^3} \left[(1+\cos\theta)S(\mathbf{q},\omega) + \ \mathbf{C_A^2}(\mathbf{3}-\cos\theta)\mathcal{S}(\mathbf{q},\omega)\right]$$

where S and $\mathcal{S}$ are the density (Fermi) and spin (Gamow Teller) response, respectively



Both long and short range correlations are important.

A Lovato, O. Benhar, S. Gandolfi & C. Losa, PRC 89, 025804 (2014)

Perspectives

- Inclusion of explicit π and Δ degrees of freedom in many-nucleon AFDMC calculations

- Use of AFDMC calculations in the interpretation of current large m_π LQCD calculations via π-less EFT. ("Effective Field Theory for Lattice Nuclei", N.Barnea, L.Contessi, D. Gazit, F. Pederiva, U. van Kolck, arXiv:1311.4966)

- Development of general formulations of DMC in Fock-space (e.g. in momentum space), to be used with strongly non-local Hamiltonians (e.g. χ-EFT-based potentials), and wave functions derived from Coupled Cluster theory (useful in quantum chemistry and materials science). (Quantum Monte Carlo with coupled-cluster wave functions"Alessandro Roggero, Abhishek Mukherjee, and Francesco Pederiva Phys. Rev. B 88, 115138 (2013))

- Search for improved algorithms based on the propagation of multiplets of points in configuration space in order to eliminate the systematic bias due to the fixed-node/fixed-phase approximations.

Thanks!

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An alternative: AFDMC

- **The crucial advantage of AFDMC** is that the scaling of the required computer resources is no longer exponential, **but scales as A^3** (the scaling required by the computation of the determinants in the antisymmetric wave functions) ➡ **LARGER SYSTEMS ACCESSIBLE!**

- **Non trivial technical issues** make the method still non optimal with respect to the standard approach for small systems.

- **ACCURATE COMPUTATIONS FOR NUCLEAR/NEUTRON MATTER FEASIBLE!**

An alternative: AFDMC

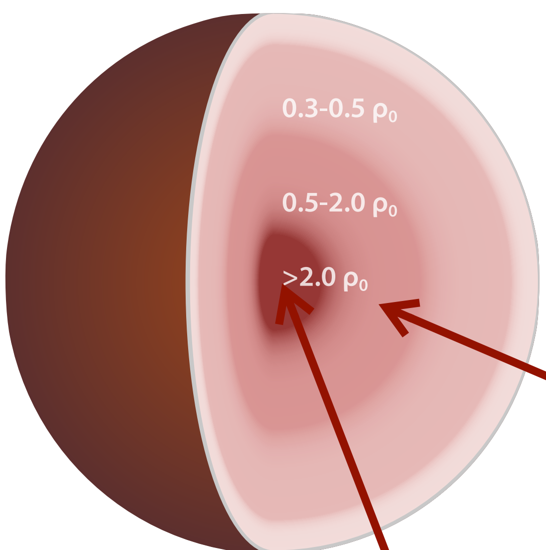
The crucial advantage of AFDMC is that the scaling of the required computer resources is no longer exponential, **but goes as *A^3*** (the scaling required by the computation of the determinants in the antisymmetric wave functions) → **LARGER SYSTEMS ACCESSIBLE!**

Problems

- Progress! The HS transformation can be used ONLY FOR THE PROPAGATOR → No possibility of using accurate wave functions that require an operatorial dependence! → Constraints used to cope with the sign problem less accurate.
- Progress! Extra variables → larger fluctuations and autocorrelations.
- Progress! Some problems in treating nuclear spin-orbit.
- Three-body forces (extremely important in nuclear physics) can be reduced by a HS transformation only for pure neutron systems.

Neutron stars

neutron star



electrons

ions

outer crust: $e \; Z$

$(0.3 \div 0.5\,\mathrm{km})$

inner crust: $e \;\; Z \;\; n$

$(1 \div 2\,\mathrm{km})$

outer core: $n \;\; p \;\; e \;\; \mu$

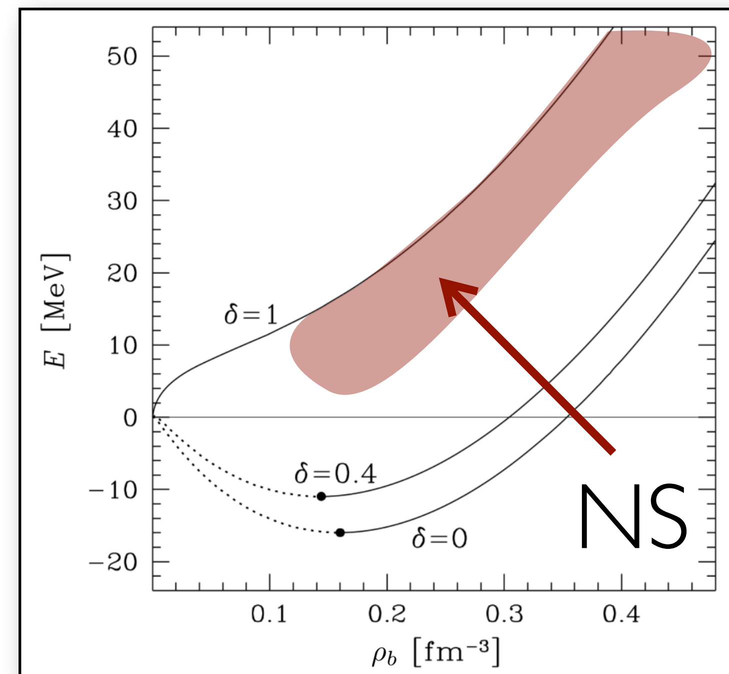
$(\sim 9\,\mathrm{km})$

inner core: n,p,e,μ **and maybe hyperons…**

$(0 \div 3\,\mathrm{km})$

$R \sim 10\,\mathrm{km}$

$M \sim 1.4\,M_\odot$



P. Haensel, A.Y. Potekhin, D.G. Yakovlev, Neutron Stars I, Springer 2007

The structure of a neutron star can be determined by solving a set of equations describing the equilibrium between the competing effects of the gravitational force (tending to make the star collapse) and the neutron-neutron (or more generally baryon-baryon) interaction that at high density provides mutual repulsion among the particles.
(Tolman-Oppenheimer-Volkov equations).

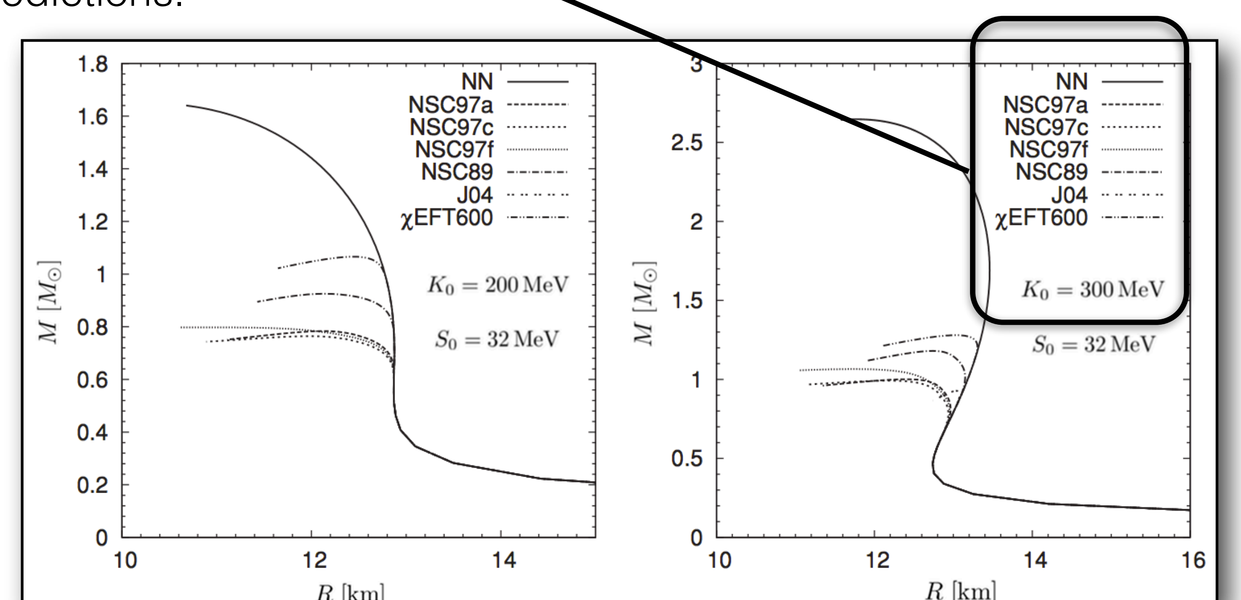
Necessary ingredient for NS theory:
energy and pressure vs. density for dense matter!

Hyperon puzzle

The appearance of hyperons (particles including a strange quark) has an immediate consequence on the equation of state: it makes it **softer**, i.e. the pressure coming from the baryon-baryon interaction is reduced. This is due to the **larger mass** and to the fact that nucleons transforming into hyperons become **distinguishable** in the Fermi sea

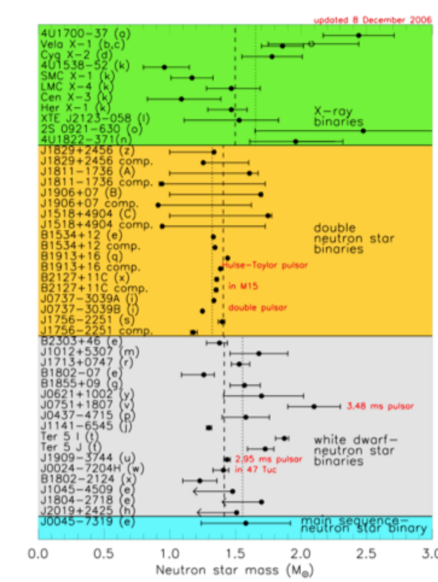
Many hyperon-nucleon model interactions, giving differen EoS and different predictions.

Softer EoS ➠ lower star mass



H. Đapo, B.-J. Schaefer, and J. Wambach. Appearance of hyperons in neutron stars. Phys. Rev. C, 81(3): 035803 (2010) based on NN ("soft" and "stiff") EoS from M.Heiselberg, M.Hjort-Jensen, Phys. Rep. 328, 237 (2000)

Until 2010 observed masses of NS were distributed around the Chandrashekar mass M_S=1.4 M⊙



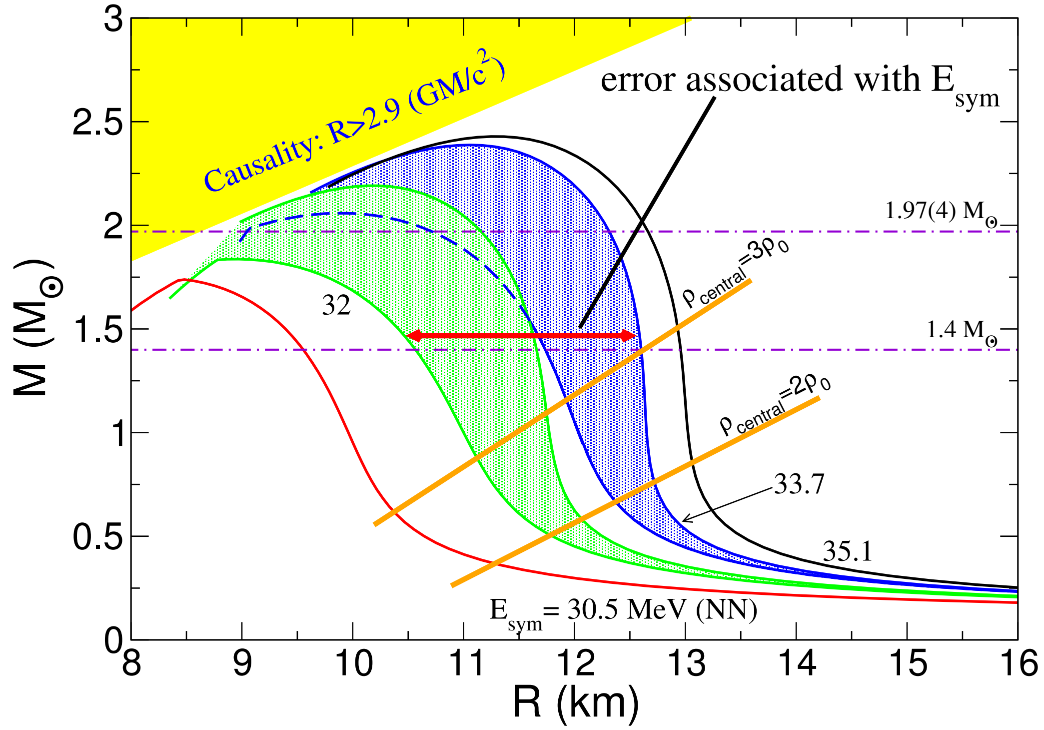
Use of the equation of state of a p,n,e,μ leads to a maximum mass > 2 M⊙

Soft EoS allowed: hyperons ok!

Hyperon Puzzle

Recently a few NS with a large mass were observed. The first (2010) was PSR~J1614-2230 pulsar with **M=1.97(4)M⊙**.

(P. B. Demorest, T. Pennucci, S. M. Ransom, M. S. E. Roberts and J. W. T. Hessels. A two-solar-mass neutron star measured using Shapiro delay measurements)



S. Gandolfi, J. Carlson, and Sanjay Reddy
Phys. Rev. A **83**, 041601 (2011)

Are there no hyperons in a NS???

Before 2010:
Maximum mass observed: 1.6M⊙
Maximum mass predicted without hyperons: 2.3⊙ (still ok in principle)
Maximum mass predicted with hyperons: 1.4-1.6M⊙ (good!)

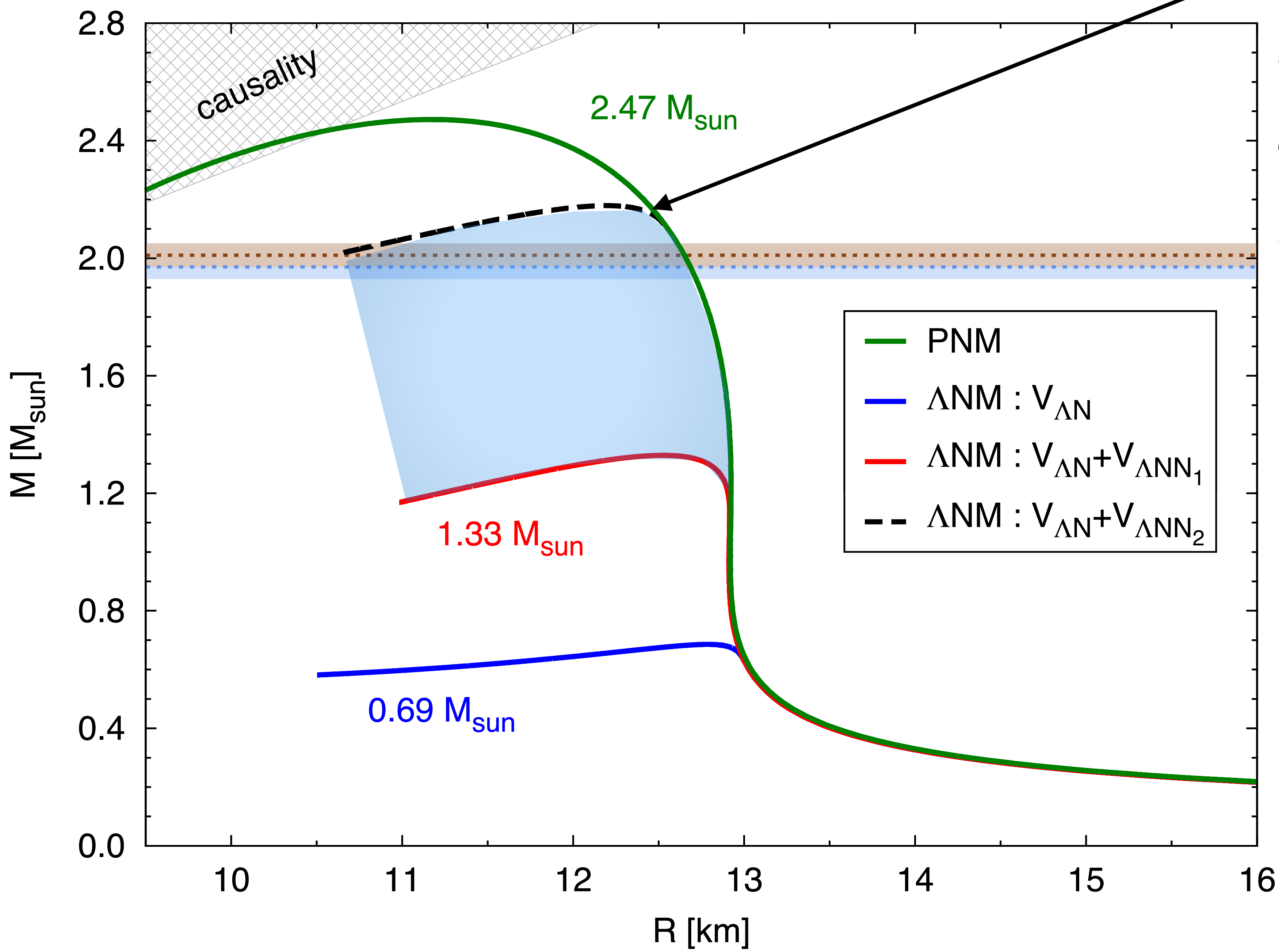
After 2010:
Observed mass: 2.0M⊙
Maximum mass predicted without hyperons: 2.3M⊙ (good!)
Maximum mass predicted with hyperons: 1.4-1.6M⊙ (very bad...)

Key problem: understand the hyperon-nucleon interaction!

NS structure

PRELIMINARY RESULT WITH THE NEW PARAMETRIZATION

Results might become compatible with the more recent astronomical observations: predicted maximum mass exceeds $2M_\odot$



D. Lonardoni, A. Lovato, S. Gandolfi, F. Pederiva

Hyperon puzzle possibly solvable!

Key to success: the possibility of performing accurate, realistic calculations for large nuclear systems.