Quantum Monte Carlo calculations of nuclear and neutron matter

Alexey Yu. Illarionov, SISSA
and coworkers:
Stefano Fantoni, SISSA
Stefano Gandolfi, SISSA
Francesco Pederiva, Trento
Kevin E. Schmidt, ASU

Outline

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- EoS: Motivations
- The AFDMC method
- EoS of nuclear matter
- EoS of neutron matter
- Superfluid low-density neutron matter
- Conclusions

Standard Model of Nuclear Physics

The main goals of the research on the SMNP model have been and still are:

- Search for a many-body nuclear interaction, capable to describe *all* the nuclear systems, from the deutron to nuclear matter up to $\rho \sim 0.5$ fm^{-3} and T of few tenths of MeV.
- Search for a current operators which are consistent with the above effective interaction (electron scattering off nuclei).
- Developments of powerful and efficient many-body methods to solve the corresponding Schrödinger equation through *ab-initio* calculations, namely those with **no** approximations on the nuclear interaction (due to short range correlations and spin problem).

EoS: Motivations

- EoS of nuclear and neutron matter relevant for nuclear astrophysics (evolution of neutron stars)
- **Theoretical uncertainties** on the calculation of symmetric EoS derive both from the *approximations* introduced in the many-body methods and from using model *interactions*
- Properties of nuclei are well described by realistic **NN** and **TNI** interactions but limited to **A=12** with GFMC technique (or less with other accurate few-body methods).

Hamiltonian

We consider *A* non-relativistic nucleons with an effective **NN** and **TNI** forces that model the pion-exchange between nucleons:

$$H = \frac{\hbar^2}{2m} \sum_{i=1}^{A} \nabla_i^2 + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk} \tag{1}$$

NN is usually written as

$$v_{ij} = \sum_{p=1}^{M} v_p(r_{ij}) O^{(p)}(i,j) \tag{2}$$

where $O^{(p)}$ are operators including spin, isospin, tensor and others. The TNI model 2- and 3-π exchange between nucleons with also some Δ excited state. The general form is

$$V_{ijk} = A_{2\pi}^{PW} O_{ijk}^{2\pi,PW} + A_{2\pi}^{SW} O_{ijk}^{2\pi,SW} + A_{3\pi}^{\Delta R} O_{ijk}^{3\pi,\Delta R} + A_R O_{ijk}^{R} \,. \tag{3}$$

The main contribution to **NN** interaction is given by **OPE**, but also other processes are included. The most important operators are

$$O_{ij}^{p=1,8} = (1, \vec{\sigma}_i \cdot \vec{\sigma}_j, S_{ij}, \vec{L}_{ij} \cdot \vec{S}_{ij}) \times (1, \vec{\tau}_i \cdot \vec{\tau}_j)\,, \tag{4}$$

where $\vec{L}_{ij}$ is the relative angular momentum, $\vec{S}_{ij}$ is the total spin, and

$$S_{ij} = 3(\vec{\sigma}_i \cdot \hat{r}_{ij})(\vec{\sigma}_j \cdot \hat{r}_{ij}) - \vec{\sigma}_i \cdot \vec{\sigma}_j\,. \tag{5}$$

The **TNI** model following processes:

For example the Fujita-Miyazawa diagram gives:

$$O_{ijk}^{2\pi,PW} = \sum_{cyc} \left[\left\{X_{ij}^{\pi}, X_{jk}^{\pi}\right\} \left\{\tau_i \cdot \tau_j, \tau_j \cdot \tau_k\right\} + \frac{1}{4}\left[X_{ij}^{\pi}, X_{jk}^{\pi}\right]\left[\tau_i \cdot \tau_j, \tau_j \cdot \tau_k\right] \right], \tag{6}$$

DMC for central potentials

A generic trial wave function can be expanded

$$\psi_T(R) \equiv \psi(R,0) = \sum_n c_n \phi_n(R)\,, \tag{7}$$

and the formal solution of a Schrödinger equation in imaginary time $\boldsymbol{\tau}$ is given by:

$$\begin{aligned}\psi(R,\tau) &= e^{-(H-E_T)\tau}\psi(R,0) = \\ &= e^{-(E_0-E_T)\tau} c_0\psi_0(R,0) + \sum_{n\neq 0} e^{-(E_n-E_T)\tau} c_n\phi_n(R,0)\end{aligned}$$

In the limit of $\tau \to \infty$ it converges to the lowest energy eigenstate not orthogonal to $\psi(R,0)$.

DMC for central potentials

The imaginary-time Schrödinger equation = diffusion + rate processes

$$\frac{\partial\psi(R,\tau)}{\partial\tau} = D\nabla^2\psi(R,\tau) + (E_T - V(R))\psi(R,\tau). \qquad (8)$$

The propagation is performed by means of the integral equation

$$\psi(R,\tau) = \langle R|\psi(\tau)\rangle = \int dR' G(R,R',\tau)\psi(R',0) \qquad (9)$$

The propagator is written explicitly **only** for short times:

$$\begin{aligned} G(R,R',\Delta\tau) &= \langle R|e^{-H\Delta\tau}|R'\rangle = \\ &= \left(\frac{m}{2\pi\hbar^2\Delta\tau}\right)^{\frac{3A}{2}} e^{\frac{-m(R-R')^2}{2\hbar^2\Delta t}} e^{-\left[\frac{V(R)+V(R')}{2} - E_T\right]\Delta\tau} + O(\Delta\tau^3) \end{aligned}$$

Then we need to iterate many times the above integral equation in the small time-step limit.

DMC and nuclear Hamiltonians

The DMC technique is easy to apply when the interaction is purely central.

For realistic NN potentials, the presence of quadratic spin and isospin operators in the propagator imposes the summation over all the possible good spin-isospin single-particle states because

$$(\vec{\sigma}_1 \cdot \vec{\sigma}_2)\,|\uparrow_1\downarrow_2\uparrow_3\rangle = \alpha|\uparrow_1\downarrow_2\uparrow_3\rangle + \beta|\downarrow_1\uparrow_2\uparrow_3\rangle \tag{10}$$

This is the approach of the **GFMC** of Pieper et al., including a huge number of states in the wave function:

$$\# \approx \frac{A!}{Z!(A-Z)!}2^A \tag{11}$$

The basic idea of AFDMC is to sample spin-isospin states instead of the explicit summation.

The application to **pure neutron** systems is due to Schmidt and Fantoni[1].

Unfortunately, the extension to proton-neutron systems interacting with some tensorial force was unexpectedly difficult.

[1] K.E. Schmidt and S. Fantoni, Phys. Lett. 445, 99 (1999)

The method consists in using the Hubbard-Stratonovich transformation in order to **reduce** the spin-isospin operators in the Green's function from quadratic to linear:

$$e^{\frac{1}{2}\Delta t O^2} = \frac{1}{\sqrt{2\pi}} \int dx e^{-\frac{x^2}{2} + x\sqrt{\Delta t} O} \qquad (12)$$

Auxiliary Field DMC: Diagonalization

The spin-isospin dependent part of NN interaction can be written as:

$$v_{SID} = \frac{1}{2} \sum_{i\alpha, j\beta} \sigma_{i\alpha} A_{i\alpha, j\beta} \sigma_{j\beta} \vec{\tau}_i \cdot \vec{\tau}_j = \frac{1}{2} \sum_{\alpha=1}^{3} \sum_{n=1}^{3A} \hat{S}_{n\alpha}^2 \lambda_n \,, \qquad (13)$$

where A is a real and symmetric matrix containing the interaction between nucleons, λ are the real eigenvalues of A, and $\hat{S}$ are operators written in terms of eigenvectors of A:

$$\hat{S}_{n\alpha} = \sum_i \tau_{i\alpha} \vec{\sigma}_i \cdot \vec{\psi}_n(i) \,. \qquad (14)$$

The Hubbard-Stratonovich transformation is applied to the Green's function for the spin-isospin dependent part of the potential:

$$e^{-v_{SID}\Delta t} \cong \prod_{n=1}^{(3+9+3)A} e^{-\frac{1}{2}\lambda_n \hat{S}_n^2 \Delta t}, \qquad (15)$$

and

$$e^{-\frac{1}{2}\lambda_n \hat{S}_n^2 \Delta t} = \frac{1}{\sqrt{2\pi}} \int dx_n e^{-\frac{x_n^2}{2} + \sqrt{-\lambda_n \Delta t} x_n \hat{S}_n}. \qquad (16)$$

The x_n are auxiliary variables to be sampled. The effect of the $\hat{S}_n$ is a rotation of the four-component spinors of each particle (written in the proton-neutron up-down basis) without mixing the spin-isospin states of nucleon pairs.

Price to pay: diagonalization of A & sampling over x_n.

Auxiliary Field DMC: Trial wave function

The trial wave function used for the projection has the following form:

$$\psi_T(R,S) = \Phi_J(R) \cdot A[\phi_i(\vec{r}_j, s_j)] \tag{17}$$

where $R = (\vec{r}_1 ... \vec{r}_A)$, $S = (s_1 ... s_A)$ and $\{\phi_i\}$ is a single-particle base. $\Phi_J(R)$ is a Jastrow (scalar) factor:

$$\Phi_J(R) = \prod_{i<j} f(r_{ij}) \tag{18}$$

– to reduce the energy variance (does not influence the result).

Spin-isospin states are written as complex four-spinor components:

$$s_i \equiv \begin{pmatrix} a_i \\ b_i \\ c_i \\ d_i \end{pmatrix} = a_i|p\uparrow\rangle + b_i|p\downarrow\rangle + c_i|n\uparrow\rangle + d_i|n\downarrow\rangle \,,$$

Auxiliary Field DMC: Additional items

- Importance sampling: in order to decrease the variance on the estimators sample from the modified Green's function

$$\tilde{G}(R, R', \Delta t) = \frac{\psi_I(R')}{\psi_I(R)} G(R, R', \Delta t)\,, \tag{19}$$

the projected distribution is $\Psi(R) = \psi_I(R)\phi_0(R)$.

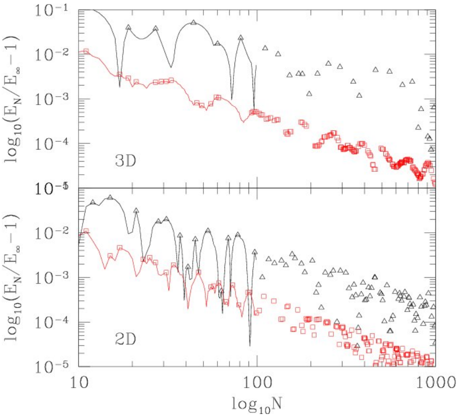
- Fermion sign problem: we artificially constrain the Ψ to be positive.
  - for real functions $\longrightarrow$ fixed-node: $\psi_I(R) > 0$ (not our case).
  - for complex functions $\longrightarrow$ constrained-path or fixed-phase.
    1. Constrained-path: $Re[\psi_I(R)] > 0$ (previously used).
    2. Fixed-phase: $\psi_I(R) = |\psi_I(R)|e^{i\Phi_I(R)}$ and we impose $\Phi(R, t) = \Phi_I(R)$ (never well tested before this work). The projected distribution is $\Psi(R) = |\psi_I(R)||\phi_0(R)|$.

- Twist-averaged boundary conditions: go beyond the closed shells

$$\psi(\vec{r}_1 + L\hat{x}, \vec{r}_2, \ldots) = e^{i\theta_x}\psi(\vec{r}_1, \vec{r}_2, \ldots), \quad -\pi < \theta_i \leq \pi \tag{20}$$

The wave vectors obey ($\vec{n}$ is an integer vector):

$$\vec{k}_n = (2\pi\vec{n} + \theta)/L.$$



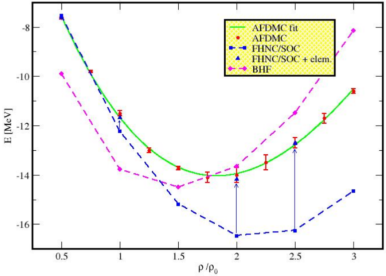
Relative error of the energy versus number of particles with PBC (△) and TABC (□) in 2D and 3D. The points shown are only those where the relative error has a local maximum. Curves are shown only for $N < 100$.

Nuclear and neutron matter

- The Jastrow factor Φ_J is a product of two-body factors related to the scalar component of the NN interaction
- Calculations were performed with nucleons in a periodic box for several densities.
- Single-particle orbitals are plane waves.
- Inclusion of some effects to correct finite-size of the system, and check of the scaling of the energy with 28, 76 and 108 nucleons (within **3%** of the total energy).
- TABC scaling check.

Nuclear Matter

The energy of 28 nucleons interacting by Argonne AV8' cut to v6' was computed for several densities[2], and compared with those given by FHNC/SOC and BHF calculations[3]:



Wrong prediction of equilibrium density ρ_0=0.16 fm^{-3} (expected for the absence of TNI).

[2] Gandolfi *et al.*, Phys. Rev. Lett. 98, 102503 (2007)

[3] Bombaci *et al.*, Phys. Lett. B 609, 232 (2005)

Neutron matter

The same calculation performed with GFMC was repeated[4]. Using the Argonne AV8' in the Hamiltonian, the energy of 14 neutrons in a periodic box is:

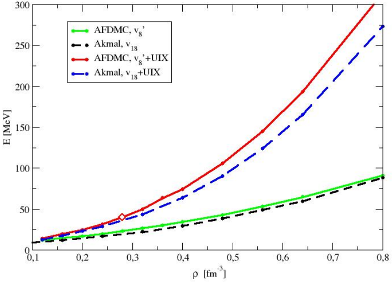
ρ [fm^{-3}]	FP-AFDMC	CP-GFMC	UC-GFMC	CP-AFDMC
0.04	6.69(2)	6.43(01)	6.32(03)	
0.08	10.050(8)	10.02(02)	9.591(06)	
0.16	17.586(6)	18.54(04)	17.00(27)	20.32(6)
0.24	26.650(9)	30.04(04)	28.35(50)	

The fixed-phase approximation improves the agreement with GFMC.

[4] Carlson *et al.*, Phys. Rev. C 68, 25802 (2003)

Neutron matter

We use the realistic nuclear Hamiltonian AV8'+UIX and 66 neutrons in a periodic box. The AFDMC EoS[5] is compared with the FHNC/SOC one of Akmal, Pandharipande and Ravenhall[6].



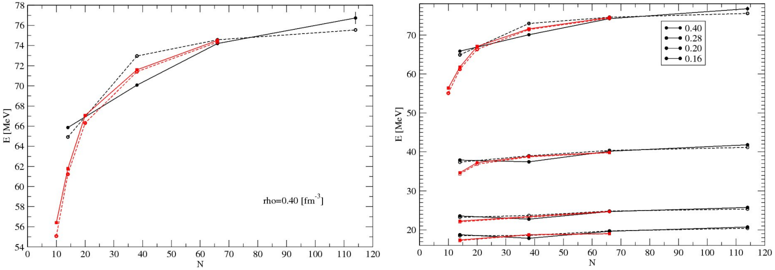
The FHNC/SOC seems to overestimate the TNI contribution (elementary diagrams in TNI evaluation?).

[5] Gandolfi *et. al.*, in preparation

[6] Akmal *et al.*, Phys. Rev. C 58, 1804 (1998)

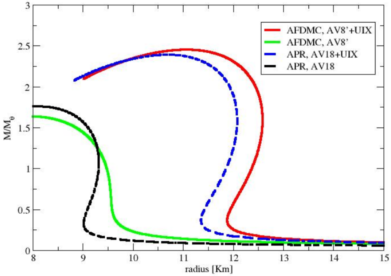
Neutron matter: Twist-averaged boundary conditions

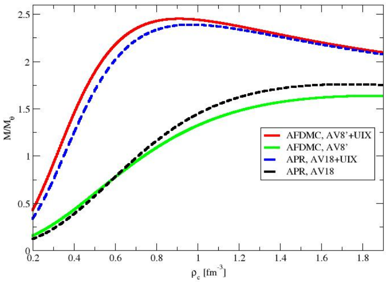
We use the TABC to control the finite-size effects and to perform the calculations with an open shell systems.



Neutron star structure

We solved the TOV equation to compare the structure of the star predicted by AFDMC-EoS and the APR one.





The less hardness predicted by APR essentially does not change the structure of the star.

Pairing in neutron star matter

AIM: Benchmark the microscopic calculations of pairing gaps

RELEVANCE: Thermodynamic & transport properties of n* matter, reflected in neutrino cooling & rotational dynamics (pulsar timing)

EXPECTATIONS: most relevant nucleonic pairing channels $\leftrightarrow$ most attractive phase-shift at given density $E \sim \rho^{2/3}$

- $^1S_0$ neutron pairing in the inner crust
- $^3P_2 - ^3F_2$ neutron pairing in the quantum fluid interior (richness of phases)
- $^1S_0$ proton pairing in the quantum fluid interior

DIFFICULTY: Exponetial sensitivity of pairing gaps to the interaction and self-energy. The BCS weak-couplin formula

$$\Delta \sim \exp\left[-1/N(0)g\right]$$

is **NOT** raliable!

"Polarization effects"

Superfluid neutron matter

- We consider the full Hamiltonian AV8'+UIX.
- The Jastrow factor is the same of that used for neutron matter.
- The antisymmetric part of the trial wave function has a *BCS* structure :

$$\Phi_{BCS} = A[\phi(\vec{r}_1, s_1, \vec{r}_2, s_2)...\phi(\vec{r}_i, s_i, \vec{r}_j, s_j)\psi_{\vec{k}}(\vec{r}_l)] \qquad (21)$$

  The pairing orbitals have the form

$$\phi(\vec{r}_{ij}, s_i, s_j) = \sum_\alpha c_\alpha e^{i\vec{K}_\alpha \cdot \vec{r}_{ij}} \xi_S(s_i, s_j) \qquad (22)$$

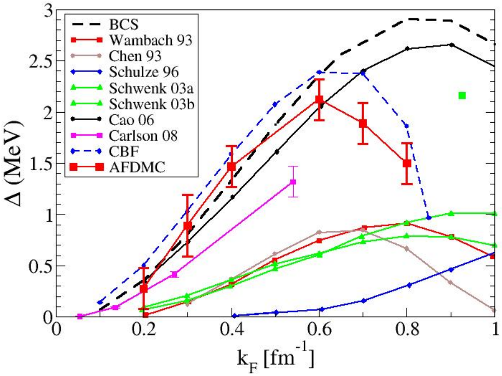
  and the c_α parameters are determined with a **CBF** calculation[7]. The unpaired orbitals, needed for odd number of neutrons, are plane waves.
- The superfluid gap is evaluated from even-odd staggering of estimated energies:

$$\Delta(N) = E(N) - [E(N+1) + E(N-1)]/2\,. \qquad (23)$$

[7] A. Fabrocini *et al.*, Phys. Rev. Lett. 95, 192501 (2005)

Comparison of predictions for singlet-S gap

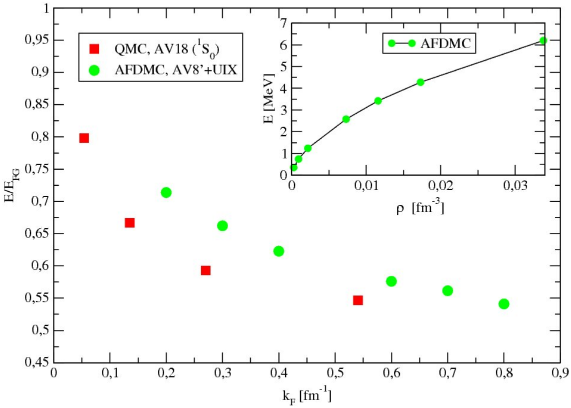
We computed the superfluid gap considering $N = 12...18$ and $N = 62...68$ neutrons[8]. The dependence of the gap by N is the same observed by Carlson with a simpler QMC calculation [9].



[8]Gandolfi *et al.*, arXiv:0805.2513, Phys. Rev. Lett. in print

[9]A. Gezerlis and J. Carlson, Phys. Rev. C 77, 032801(R) (2008)

Superfluid neutron matter: low-density EoS

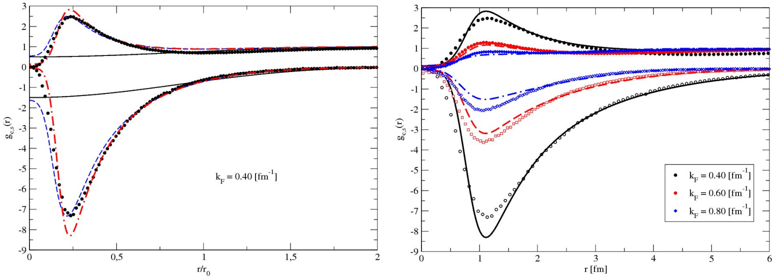


EoS of neutron matter in unit of non-interacting Fermi gas energy, as given by AFDMC for AV8′+UIX, compared with QMC results of Gerzelis and Carlson (2008) [10], considered a much simpler (central type) Hamiltonian.

[10] Gezerlis and Carlson, Phys. Rev. **C77**, 032801 (2008)

Non-interacting Fermi gas radial distributions:

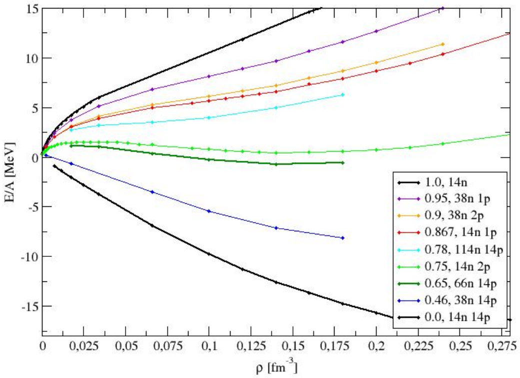
$$g_c(r) = 1 - \frac{1}{2} l^2(k_F r) \; ; \quad g_s(r) = -\frac{3}{2} l^2(k_F r).$$



VERY PRELIMINARY RESULTS!!

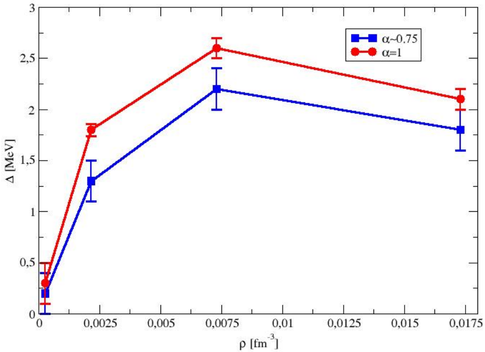
We computed the AFDMC EoS for a systems with an isospin asymmetry $\alpha = (N-Z)/(N+Z)$:

$$\frac{E(N,Z)}{A} = -a_v + a_{sym}\frac{(N-Z)^2}{A^2} \tag{24}$$



EVEN MORE PRELIMINARY RESULTS!!

We computed the superfluid gap by considering $N = 12 \ldots 18$ **paired** neutrons and 2 **unpaired** protons in the trial wave function. We are interested to see the effect of the isospin asymmetry $\alpha = \frac{N-Z}{N+Z}$ to the $^1S_0$ gap in neutron matter.



Conclusions

- AFDMC useful to study properties of neutron matter with a realistic Hamiltonian, and nuclear matter with a semi-realistic Hamiltonian.
- We revisited the EoS of neutron matter. The APR EoS seems to overestimate the TNI contribution, then TNI cannot be correctly determined using based-FHNC/SOC techniques (at least at high densities).
- The $^1S_0$ superfluid gap has been accurately computed including the full Hamiltonian rather then some effective interaction, and compared with results of other many-body techniques less accurate. The isospin-asymmetry effect to the gap is under investigation.

Present and planned future works, and perspectives

- Study of the *nn* and *np* gaps in symmetric nuclear matter (in progress).
- Inclusion of the full AV18 in the neutron matter Hamiltonian, and of spin-orbit and TNI in nuclear matter ('fake' nucleons), (in progress).
- Study of the density dependence in the Hamiltonian.
- Investigation of many-body forces in neutron and nuclear matter (follows the two previous points).
- Study of the $^3P_2 -^3 F_2$ pairing in neutron matter.
- Study exotic phases in low density nuclear matter (phase of nuclei in the matter).
- Study of neutron matter EoS with the addition of hyperons.
- Study of a new Illinois TNI to correct previous wrong versions, and maybe to be useful in neutron matter calculations (in collaboration with S. C. Pieper, ANL).