Microscopic calculation of the ⟨low-temperature⟩ equation of state of dense matter and neutron star structure

FHNC/CBF & AFDMC

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S. Gandolfi, AYuI, . . . Mon. Not. Roy. Astron. Soc. **404** (2010) L35–L39.

S. Gandolfi, AYuI, . . . Phys. Rev. **C79** (2009) 054005.

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Motivations

- $\rho < 4\rho_0$ and $T < 40$ MeV is at present completely unaccesible to QCD.
- Quantum Monte Carlo methods (GFMC and AFDMC) provide very accurate results for nuclear systems with $A \sim 100$.
- NN scattering data and few-body theory $\rightarrow$ nuclear Hamiltonians. Few-body $\rightarrow$ many-body $\rightarrow$ experiments/observations?
- EoS of nuclear and neutron matter relevant for nuclear astrophysics (neutron stars and supernovae).
- Temperature effects on the equation of state?!

Many-body methods used: AFMDC & CBF/FHNC

AFDMC ($T = 0$)

- Diffusion Monte Carlo
- Hubbard-Startonovich transformation

$$G(\mathbf{R}, \mathbf{R}', \Delta\tau) = \left(\frac{m}{2\pi\hbar^2\Delta\tau}\right)^{\frac{3A}{2}} \exp\left[-\frac{m|\mathbf{R}-\mathbf{R}'|^2}{2\hbar^2\Delta\tau}\right] e^{-V_{\mathrm{SI}}(\mathbf{R})\Delta\tau} \times \prod_{n=1}^{3A} \int \frac{dx_n}{\sqrt{2\pi}} \exp\left[-\frac{x_n^2}{2}\right] \exp\left[\sqrt{-\lambda_n\Delta\tau}\, x_n \widehat{O}_n\right]$$

- Convergence: Importance sampling
- Size problem: fixed-phase approximation
- Finite box (finite N): solved (TABC)
- v_{LS}: only neutron matter at present

CBF/FHNC ($T \geq 0$)

$$\Psi_i\left[n_i(\mathbf{k})\right] = \mathcal{S}\left(\prod_{i<j} \mathcal{F}_{ij}\right) \Phi_i\left[n_i(\mathbf{k})\right]$$

The pair correlation operator $\mathcal{F}_{ij}$:

$$\mathcal{F}_{ij} = \sum_{c, c\tau, s, s\tau, t, t\tau} f_p(r_{ij}) O_{ij}^p .$$

The Gibbs-Bogoliubov variational principle

$$F(\rho, T) \leq F_V(\rho, T) = \mathrm{Tr}\left(\rho_V H\right) - T S_V(\rho, T),$$

Fermi-Hypernetted chain equations used to evaluate

$$\frac{E_V(\rho, T)}{A} = \frac{\hbar^2 k_{\mathrm{av}}^2}{2m} + \sum \text{diagrams}\left(V, \mathcal{F}, \ell(r, \rho, T)\right)$$

- SOC $\sim \rho^2$: variational violation
- Elem. diagrams $\sim \rho^3$: sum rule control
- v_{LS} at the *second order* only

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AFDMC ($T = 0$)

- Diffusion Monte Carlo
- Hubbard-Startonovich transformation

$$
\begin{aligned}
&G(\mathbf{R}, \mathbf{R}', \Delta\tau) \\
&= \left(\frac{m}{2\pi\hbar^2\Delta\tau}\right)^{\frac{3A}{2}} \exp\left[-\frac{m|\mathbf{R}-\mathbf{R}'|^2}{2\hbar^2\Delta\tau}\right] e^{-V_{\mathrm{SI}}(\mathbf{R})\Delta\tau} \\
&\times \prod_{n=1}^{3A} \int \frac{dx_n}{\sqrt{2\pi}} \exp\left[-\frac{x_n^2}{2}\right] \exp\left[\sqrt{-\lambda_n \Delta\tau} x_n \widehat{O}_n\right]
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A generic trial wave function can be expanded

$$\psi_T(R) \equiv \psi(R,0) = \sum_n c_n \phi_n(R)\,, \tag{1}$$

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

$$\psi(R,\tau) = e^{-(H-E_T)\tau}\phi(R,0) =$$

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

In the limit of $\tau \to \infty$ it converges to the lowest energy eigenstate $\phi_0(R)$ not orthogonal to $\psi(R,0)$.

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The imaginary-time Schrödinger equation = diffusion + rate processes

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

The propagation is performed by means of the integral equation

$$\psi(R,\tau) = \langle R|\psi(\tau)\rangle = \int dR' G(R,R',\tau)\psi(R',0) \tag{3}$$

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

$$G(R,R',\Delta\tau) = \langle R|e^{-(\hat{H}-E_T)\Delta\tau}|R'\rangle =$$

$$= \left(\frac{m}{2\pi\hbar^2\Delta\tau}\right)^{\frac{3A}{2}} e^{-\frac{m(R-R')^2}{2\hbar^2\Delta t}} e^{-\left[\frac{V(R)+V(R')}{2} - E_T\right]\Delta\tau} + O(\Delta\tau^3)$$

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

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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

$$(\vec{\sigma}_1 \cdot \vec{\sigma}_2)\,|\uparrow_1\downarrow_2\uparrow_3\rangle = \alpha|\uparrow_1\downarrow_2\uparrow_3\rangle + \beta|\downarrow_1\uparrow_2\uparrow_3\rangle \tag{4}$$

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

$$\# \approx \frac{A!}{Z!(A-Z)!}2^A \tag{5}$$

Auxiliary Field DMC: Hubbard-Stratonovich

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

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:

$$e^{\frac{1}{2}\Delta t O^2} = \frac{1}{\sqrt{2\pi}} \int dx e^{-\frac{x^2}{2} + x\sqrt{\Delta t} O} \qquad (6)$$

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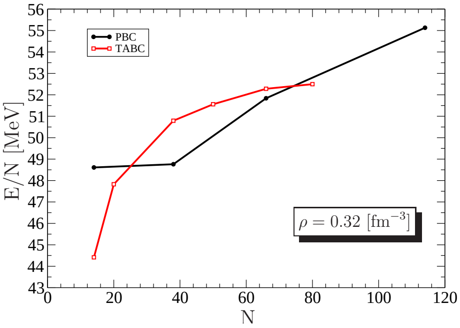

Convergence of the computed energy at $\rho = 0.32$ fm^3 as a function of neutrons in a box within the grid twist-averaging method (TABC) with ten twists: the Argonne v_8 + Urbana-IX Hamiltonian were considered. The equation of state is compared with the fixed-phase AFDMC calculations with periodic boundary conditions (PBC) shown by solid lines.

Finite-size effects are under control.

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Fixed-phase test: Neutron matter

The same calculation performed with GFMC was repeated[1]. Using the Argonne AV8′ in the Hamiltonian, the energy of 14 neutrons in a periodic box is:

ρ [fm^{-3}]	FP-AFDMC	CP-AFDMC	CP-GFMC	UC-GFMC
0.04	6.75(7)		6.43(01)	6.32(03)
0.08	10.29(1)		10.02(02)	9.591(06)
0.16	17.67(5)	20.32(6)	18.54(04)	17.00(27)
0.24	27.7(5)		30.04(04)	28.35(50)

Table: Fixed phase (FP-AFDMC) energies per particle of 14 neutrons interacting with the Argonne v_8' interaction in a periodic box without the inclusion of finite size effects at various densities. All the energies are expressed in MeV.

The fixed-phase approximation improves the agreement with GFMC.

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[1] Carlson *et al.*, Phys. Rev. **C68**, 25802 (2003)

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$$v^p_{\mathrm{DD6'}} = v^p_{\mathrm{OPEP}} + v^p_I e^{-\gamma_1 \rho} + v^p_S + \mathrm{TNA}(\rho)\,,$$
$$\mathrm{TNA}(\rho) = 3\gamma_2 \rho^2 e^{-\gamma_3 \rho} \left(1 - \frac{2}{3}\left(\frac{\rho_n - \rho_p}{\rho_n + \rho_p}\right)^2\right)$$

with γ_1, γ_2 and γ_3 being fixed by means of AFDMC method, so as to reproduce the experimental values of the saturation density $\rho_0 = 0.16$ fm^{-3}, the binding energy per particle $E_0 = -16$ MeV and the compressibility $K = 9\rho_0^2 \left(\partial^2 E(\rho)/\partial\rho^2\right)_{\rho_0} \approx 240$ MeV.
The available scattering data in S-, P-, D-, F-waves are well reproduced.

parameter	*FHNC/SOC*	*AFDMC*
γ_1	0.15 fm^3	0.10 fm^3
γ_2	-700 fm^6	-750 fm^6
γ_3	13.6 fm^3	13.9 fm^3

The $\gamma_1\rho$ term simulates the effect of the three(many)-body repulsion.
TNA(ρ) simulates an attractive many-body contribution via correlations.

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S. Gandolfi, AYuI, S. Fantoni, J.C. Miller, F. Pederiva and K.E. Schmidt
Mon. Not. R. Astron. Soc. 404, L35 (2010) [arXiv:0909.3487]

$$E_{\rm SNM}(\rho)/A = E_0 + a(\rho-\rho_0)^2 + b(\rho-\rho_0)^3 e^{\gamma(\rho-\rho_0)}\,,$$
$$E(\rho,x_p)/A = E_{\rm SNM}(\rho)/A + C_s\left(\frac{\rho}{\rho_0}\right)^{\gamma_s}(1-2x_p)^2\,.$$

Parameters: $E_0 = -16.0$ MeV, $\rho_0 = 0.16$ fm^{-3}, $a = 520.0$ MeVfm^6, $b = -1297.4$ MeVfm^9 and $\gamma = -2.213$ fm^3. $C_s = 31.3$ MeV and $\gamma_s = 0.64$.

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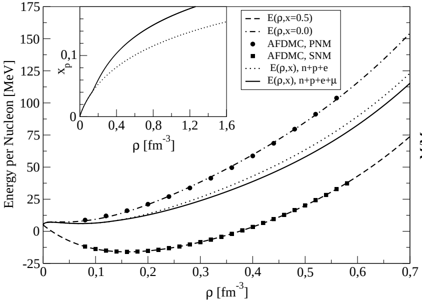

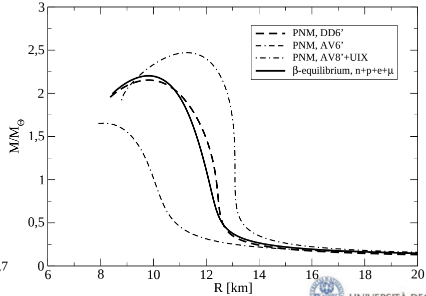

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Cold nucleon matter / Neutron star calculations

S. Gandolfi, AYuI, S. Fantoni, J.C. Miller, F. Pederiva and K.E. Schmidt
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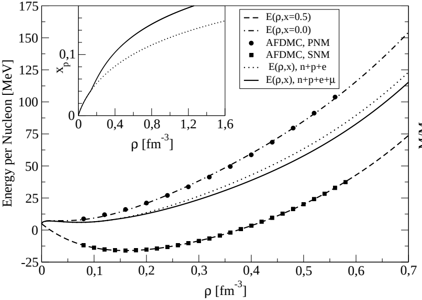

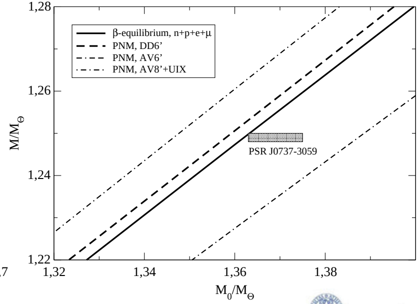

Podsiadlowski P. et al., Mon. Not. R. Astron. Soc. 361, 1243 (2005).

S. Gandolfi, AYuI, S. Fantoni, J.C. Miller, F. Pederiva and K.E. Schmidt
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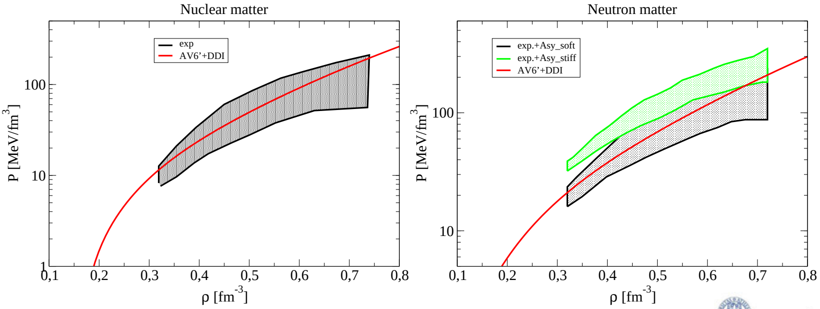

Danielewicz P., Lacey R. and Lynch W.G., Science 298, 1592 (2002).

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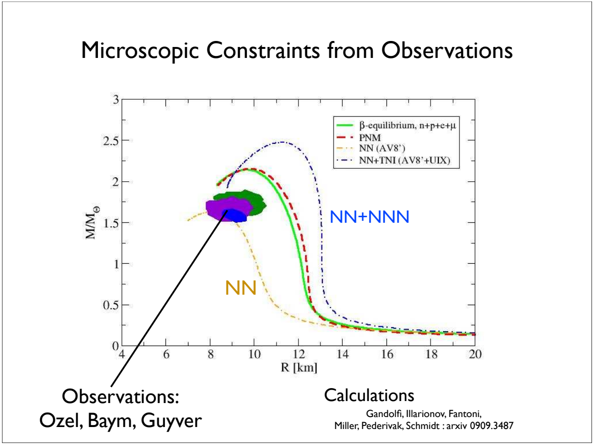
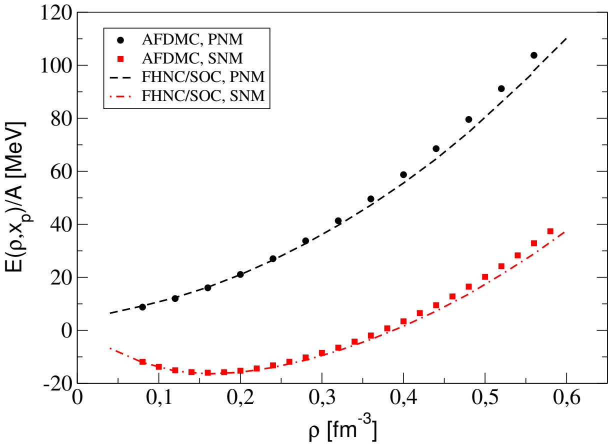


The constraned variational free energy:

$$F_{\text{con}}(\rho, T)/A = F(\rho, T)/A + \rho\Lambda \left[(I_c - 1)^2 + (I_\tau/3 + 1)^2 \right] .$$



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$$F(\rho, T, x_p)/A \approx E(\rho, x_p)/A - \alpha(x_p)\left(\frac{\rho_0}{\rho}\right)^{\beta(x_p)} T^2,$$

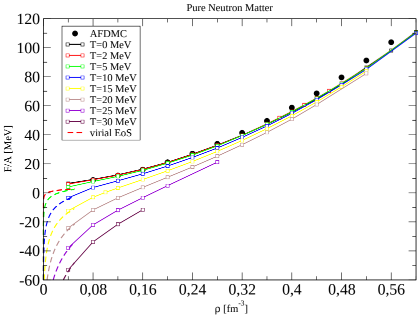
$$S(\rho, T, x_p) = -\left(\frac{\partial F/A}{\partial T}\right)_V \approx 2\alpha(x_p)\left(\frac{\rho_0}{\rho}\right)^{\beta(x_p)} T$$

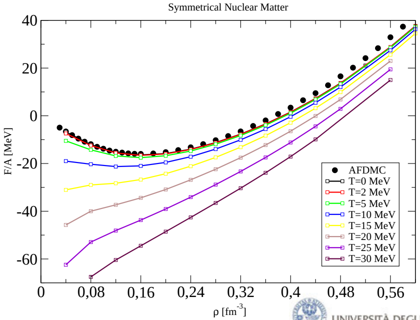
PNM: $x_p = 0$

$\alpha(0)/2^{1/3} = 0.0227, \beta(0) = 0.666$

SNM: $x_p = 1/2$

$\alpha(1/2)/4^{1/3} = 0.0253, \beta(1/2) = 0.647$





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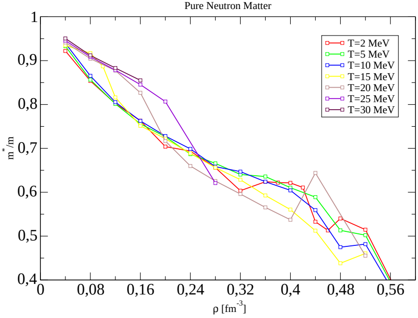
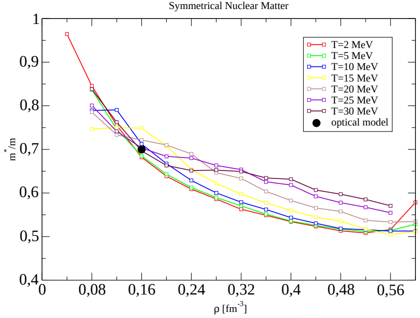
$$\epsilon(\mathbf{k},\rho,T) = \frac{\hbar^2 k^2}{2m\left[1 + A(\rho,T)\exp\left(-B(\rho,T)k^2\right)\right]}\,,\quad \frac{m^\star(\rho,T)}{m} = \frac{\hbar^2}{m}\left(\frac{1}{k}\frac{d\epsilon}{dk}\right)^{-1}_{k_F}\,,$$

$$\bar{n}(\mathbf{k},\rho,T) = \frac{1}{\exp\left[\beta\left(\epsilon(\mathbf{k},\rho,T) - \mu(\rho,T)\right)\right] + 1}\,,\ A = \sum_{\mathbf{k}} \bar{n}(\mathbf{k},\rho,T)\,.$$





Conclusions

- new EoS from microscopic calculations using the Auxiliary Field Diffusion Monte Carlo technique with nucleons interacting via a semi-phenomenological Hamiltonian (realistic 2-body + pheno many-body). LFP model revised.
- – observational constraints passed.
- first time an elementary diagrams contribution in FHNC/CBF is fully estimated $\rightarrow$ variational principle restored.
- new low-temperatire EoS from microscopic calculations using the restored FHNC/CBF technique.
  low-density limit $\rightarrow$ virial EoS, high-density limit $\rightarrow$ T^2/ρ^β.
- thermodynamics

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