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Montecarlo approach to nuclear matter.

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Monte Carlo Approach to nuclei and nuclear matter

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Outline

- The FHNC/QMC strategy
- A sketch of the AFDMC method
- Results for Nuclei
- Results on symmetric nuclear matter
- Conclusions

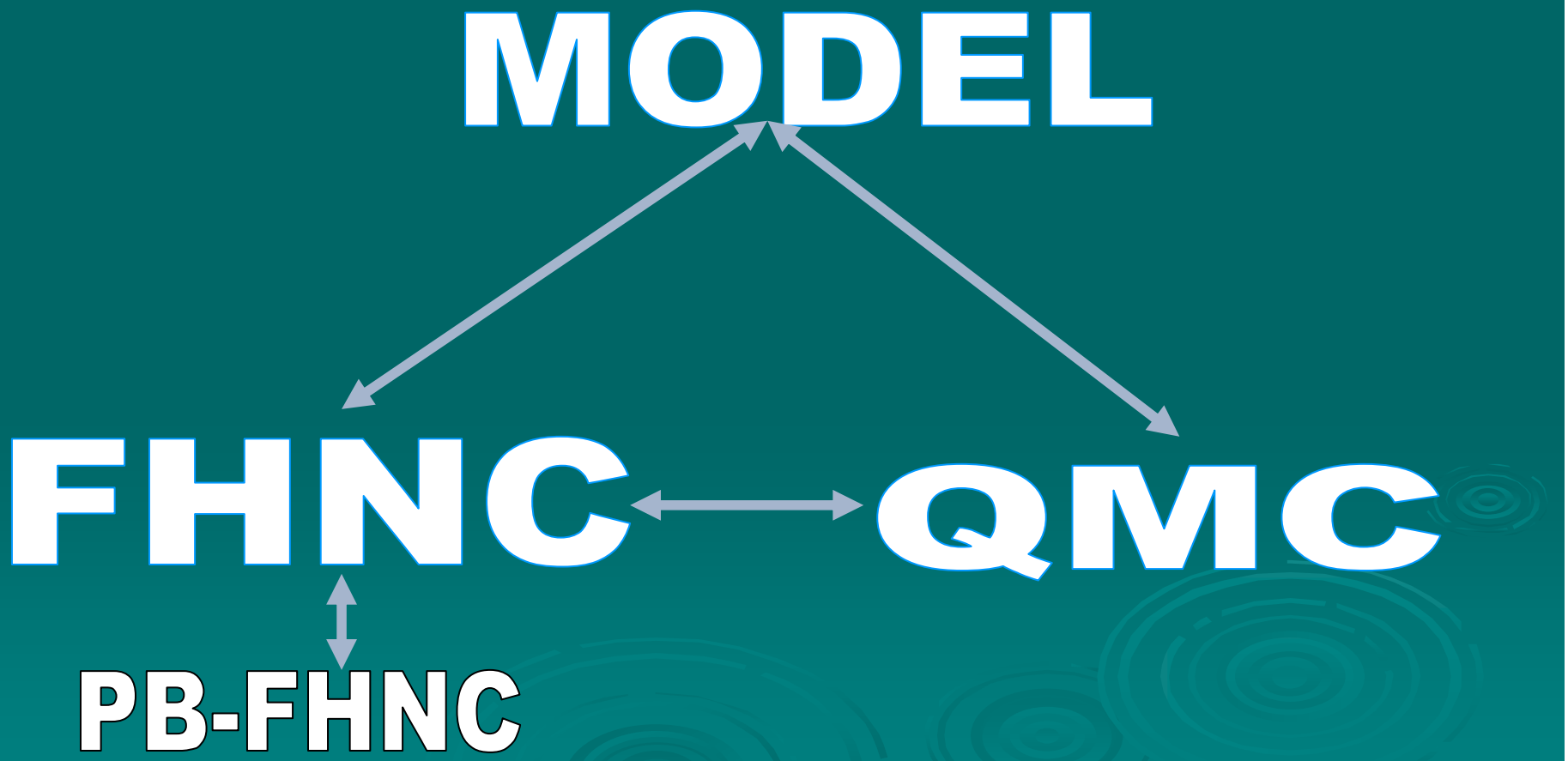
The prejudice

- Nuclear Matter is a strongly correlated fermion system which, in first approximation, can be described by a non relativistic model

The goal

- Solve the non relativistic nuclear many-body problem *without* approximations
- Test non relativistic models over the whole range of nuclear physics from light nuclei to the nuclear matter in the interior of compact stars

The theoretical method



Nuclear Hamiltonian

Let us describe our N nucleons system with the following Hamiltonian:

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \sum_{i<j} \sum_{p=1}^{M} v_p(r_{ij}) O^{(p)}(i,j) + v_{three}$$

r_{ij} is the distance between the nucleons and the $O^{(p)}$ are operators including spin, isospin, and spin-orbit operators. M is the maximum number of operators (M=18 for the Argonne v_{18} two-body potential). v_{three} is the three-body potential (for instance, Urbana IX)

Nuclear Hamiltonian

The first six operators of the two-body potential:

$$O^{p=1...6} = (\mathbf{1}, \sigma_i \cdot \sigma_j, S_{ij}) \otimes (\tau_i \cdot \tau_j)$$

$$S_{ij} = 3(\mathbf{r}_{ij} \cdot \sigma_i)(\mathbf{r}_{ij} \cdot \sigma_j) - \sigma_i \cdot \sigma_j$$

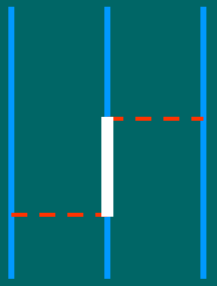
Other components include spin-orbit, quadratic spin-orbit, L^2 , charge symmetry violating terms.

Models: v_{18}, $v_{8'}$, $v_{6'}$ and $v_{4'}$

Nuclear Hamiltonian

Urbana IX three-body force $v_{three}(ijk) = S_3(ijk) + V_3(ijk)$:

$$S_3 = U_0 \sum_{cyc} T^2(r_{ij}) T^2(r_{jk})$$



$$V_3 = A \sum_{cyc} \left(\{X_{ij}, X_{jk}\} \{\vec{\tau}_i \cdot \vec{\tau}_j, \vec{\tau}_j \cdot \vec{\tau}_j\} + \frac{1}{4} [X_{ij}, X_{jk}] [\vec{\tau}_i \cdot \vec{\tau}_j, \vec{\tau}_j \cdot \vec{\tau}_j] \right)$$

$$X_{ij} = Y(r_{ij}) \vec{\sigma}_i \cdot \vec{\sigma}_j + T(r_{ij}) S_{ij}$$

DMC for central potentials

Basic observation:

The Schroedinger equation in imaginary time is a diffusion equation:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(R) - E_T\right]\Psi(R,\tau) = -\frac{\partial}{\partial\tau}\Psi(R,\tau)$$

where R represent the coordinates of the nucleons, and $\tau = it$ is the imaginary time.

DMC for central potentials

The formal solution

$$\Psi(R,\tau) = e^{-(H-E_T)\tau}\Psi(R,0)$$
$$= e^{-(E_0-E_T)\tau}c_0\Psi_0(R,0) + \sum_{n\neq 0} e^{-(E_n-E_T)\tau}c_n\Psi_n(R,0)$$

converges to the lowest energy eigenstate not orthogonal to $\Psi(R,0)$

DMC for central potentials

We can write explicitly the propagator only for short times:

$$< R \mid e^{-H\tau} \mid R' >= G(R, R', \tau) =$$

$$= \left[\frac{1}{2\tau^2} \right]^{\frac{3A}{2}} e^{-\frac{(R-R')^2}{\sigma^2}} e^{-\left[\frac{V(R)+V(R')}{2} - E_T \right] \tau}$$

$$\sigma^2 = 4 \frac{\hbar^2}{2m} \tau$$

DMC for central potentials

The $G(R,R',\Delta\tau)$ samples a population of "walkers" in configuration space.

The density of walkers is proportional to Ψ.

Expectation value of the energy is the average local energy computed over a chosen trial function Ψ_T

$$\langle H \rangle = \frac{\sum_{k=1}^{\#\ \text{walkers}} \frac{H\Psi_T(R_k)}{\Psi_T(R_k)}}{\sum_{k=1}^{\#\ \text{walkers}} 1}$$

DMC for central potentials

additional terms

- IMPORTANCE SAMPLING. In order to decrease variance on the estimators sample from

$$\frac{\Psi_T(R)}{\Psi_T(R')} G(R, R' \Delta\tau)$$

and solve for $\Psi_T(R)\Psi(R, \Delta\tau)$

- FERMION SIGN PROBLEM! The projection from an antisymmetric function either gives exponentially decaying signal or exponentially increasing noise. Use either fixed node approximation or transient estimation.

DMC and Nuclear Hamiltonians

The standard QMC techniques are easy to apply whenever the interaction is purely central, or whenever the wavefunction can be written as a product of eigenfunctions of S_z.

For realistic potentials the presence of quadratic spin and isospin operators imposes the summation over all the possible good S_z and T_z states.

$$\frac{A!}{Z!(A-Z)!}2^A$$

The huge number of states limits present calculations to A≤14

Auxiliary Fields

The use of auxiliary fields and constrained paths is originally due to S. Zhang for condensed matter problems (S.Zhang, J. Carlson, and J.Gubernatis, PRL**74**, 3653 (1995), Phys. Rev. **B55**. 7464 (1997))

Application to the Nuclear Hamiltonian is due to S.Fantoni and K.E. Schmidt (K.E. Schmidt and S. Fantoni, Phys. Lett. 445, 99 (1999))

The method consists of using the Hubbard-Stratonovich transformation in order to reduce the spin operators appearing in the Green's function from quadratic to linear.

Auxiliary Fields

For N nucleons the NN interaction can be re-written as

$$V = V_{si} + V_{sd} = V_{si} + \sum_{i\alpha;j\beta} s_{i\alpha} A_{i\alpha;j\beta} s_{j\beta}$$

where the 3Nx3N matrix *A* is a combination of the various v(p) appearing in the interaction. The *s* include both spin and isospin operators, and act on *4-component spinors:*

$$\chi_i = a_i \left| n^{\uparrow} \right\rangle + b_i \left| p^{\uparrow} \right\rangle + c_i \left| n^{\downarrow} \right\rangle + d_i \left| p^{\downarrow} \right\rangle$$

THE INCLUSION OF TENSOR-ISOSPIN TERMS HAS BEEN THE MOST RELEVANT DIFFICULTY IN THE APPLICATION OF AFDMC SO FAR

Auxiliary Fields

The matrix *A* can be diagonalized:

$$\sum_{j\beta} A_{i\alpha;j\beta}\Phi^{n}_{j\beta} = \lambda_n \Phi^{n}_{i\alpha}$$

Both eigenvectors and eigenvalues are real. This leads to the definition of a new set of operators:

$$O_n = \sum_{i\alpha} s_{i\alpha}\Phi^{n}_{i\alpha}$$

then the spin-isospin dependent part of the interaction can be expressed as

$$V_{sd} = \frac{1}{2}\sum_{n=1}^{3N} \lambda_n O_n^2$$

Auxiliary Fields

We can apply the Hubbard-Startonovich transformation to the Green's function for the spin-dependent part of the potential:

$$e^{-V_{sd}\tau} \cong \prod_{n=1}^{3N} e^{-\frac{1}{2}\lambda_n O_n^2 \tau}$$

Commutators neglected

$$e^{-\frac{1}{2}\lambda_n O_n^2 \tau} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx_n \exp\left\{-\frac{x_n^2}{2} - \sqrt{-\lambda_n \tau}\, x_n O_n\right\}$$

The x_n are auxiliary variables to be sampled. The effect of the O_n is a rotation of the spinors of each particle.

Auxiliary fields

Additional remarks

- ***Spin-orbit*** and ***three body*** terms can be treated in a similar way (with some extra care)
- ***Fermion sign problem*** still in place, with the additional difficulty of dealing with wave functions which are complex.
- using constrained-path or fixed-phase ?:
- Fixed phase has been found to be much more effective than constrained-path in dealing with tensor-tau and spin-orbit potentials.

Auxiliary fields

Technical remark

Constrained path

$$Drift = \frac{\nabla \Re \Psi_T}{\Re \Psi_T}$$

$$\Re\left(\frac{\Psi_T(R')}{\Psi_T(R)}\right) \geq 0$$

Fixed phase

$$Drift = \frac{\nabla |\Psi_T|}{|\Psi_T|}$$

$$\phi(R') = \phi(R)$$

Pure Neutron Matter

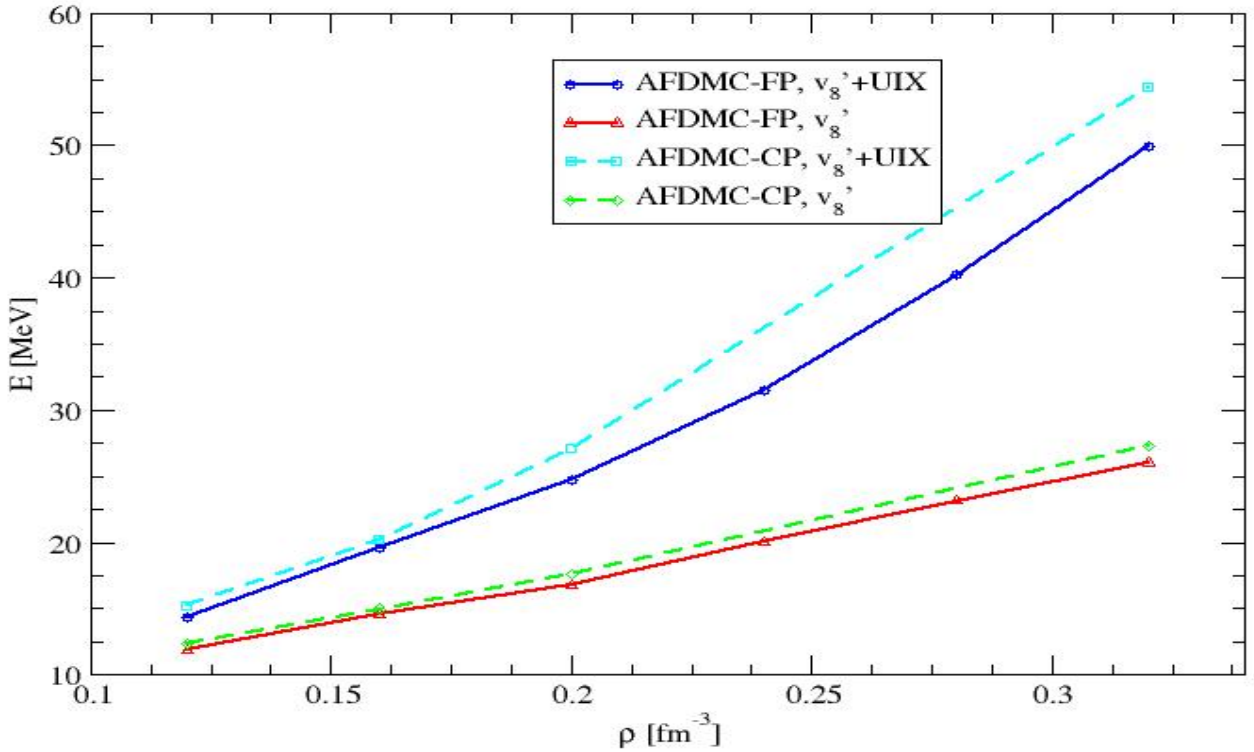
constrained path results

	ρ	N=14	N=38	N=66	N=114	N= infty
AU6'	0.12	14.96(6)	13.76(9)	14.93(4)	15.62(8)	15.0
	0.20	25.29(6)	24.4(1)	26.51(6)	27.6(1)	26.9
	0.40	69.9(1)	74.5(2)	79.4(2)	82.2(2)	81.3
AU8'	0.12	14.80(9)	13.96(5)	15.26(5)		15.5
	0.20	25.23(8)	24.7(1)	27.1(1)		27.6
	0.40	70.3(2)	76.3(2)	81.4(3)		83.5

A.Sarsa, SF, K.E.Schmidt, F.Pederiva, PRC 68,024308 (2003)
SF, K.E.Schmidt, Nucl.Phys A690, 456 (2001) [PB-FHNC]

Pure neutron Matter (66 neutrons)

fixed phase versus constrained path

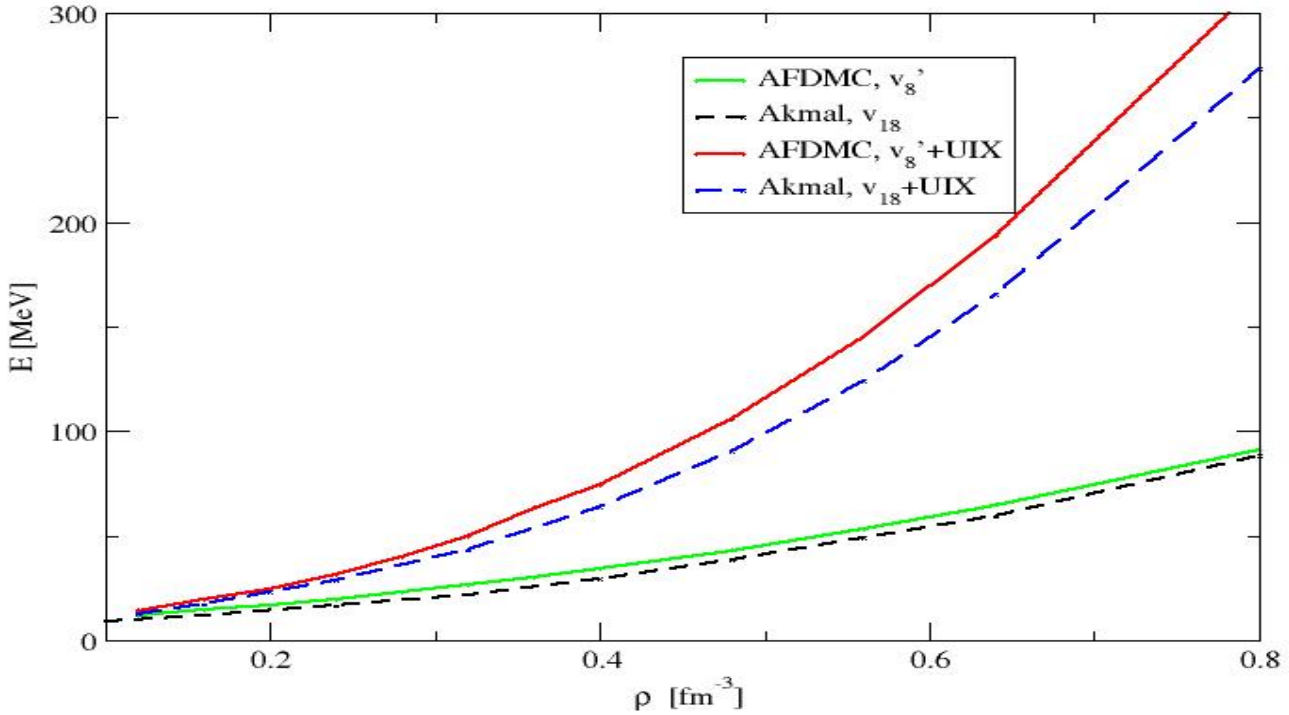


A.Sarsa, SF, K.E.Schmidt, F.Pederiva, PRC 68,024308 (2003)

S.Gandolfi et al., private communication

Pure neutron matter (66 neutrons)

AFDMC versus FHNC-SOC



S.Gandolfi et al., private communication

Pure Neutron Matter

$^1S_0$ superfluid phase (AU8' interaction)

$K_F = 0.6$ fm $^{-1}$

N	E/N	GAP
12	2.6356(17)	
13	2.7593(17)	2.182(37)
14	2.5536(15)	
15	2.8036(17)	2.855(44)
16	2.6654(18)	
17	2.8075(15)	2.333(49)
18	2.6746(17)	
		2.457(76)

With constrained path

Gap=E(N)-(E(N+1)-E(n-1))/2

FHNC/BCS versus AFDMC with Pfaffians

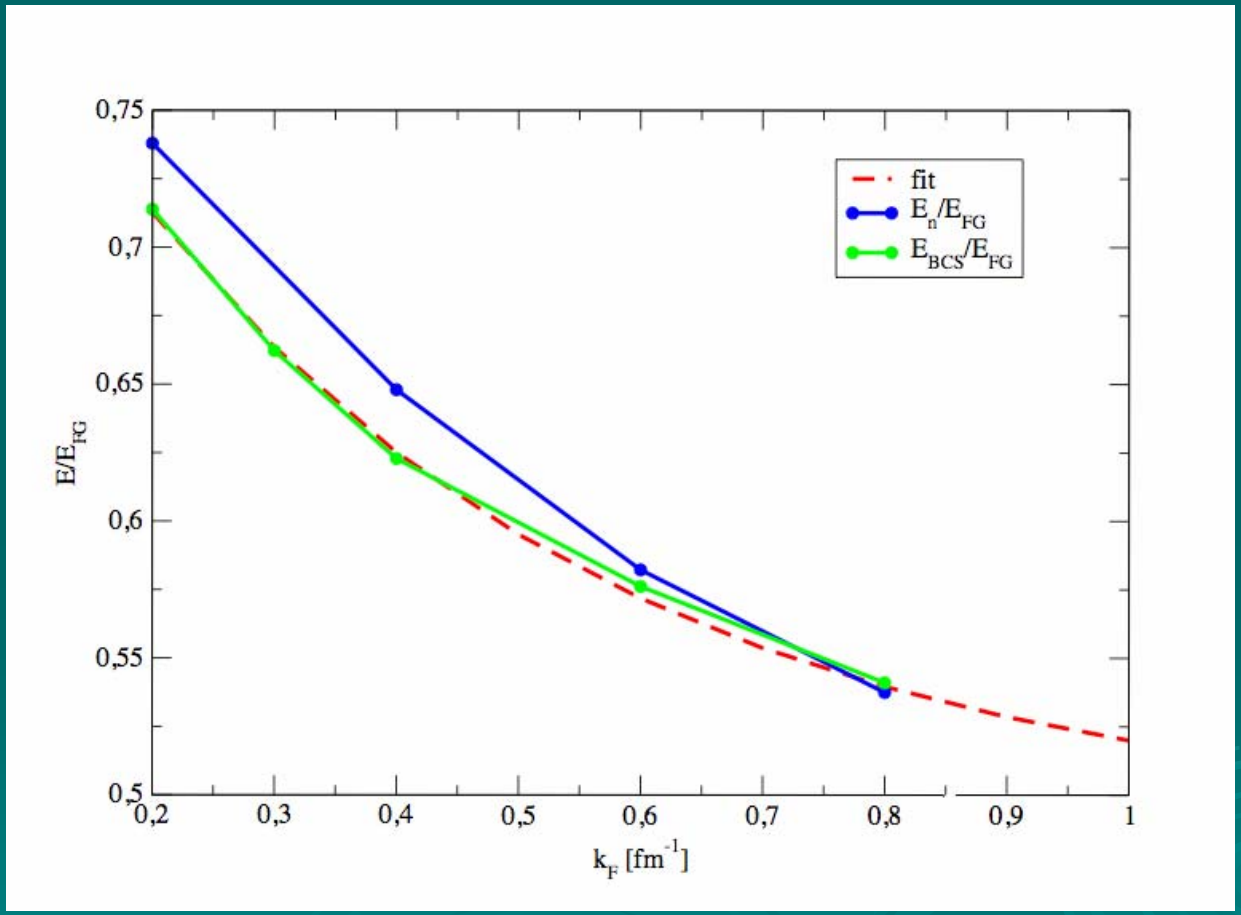
N=50-56, Gap=2.54(58)

N=62-66, Gap=2.58(55)

A.Fabrocini, SF, A.Y.Illarionov, K.E.Schmidt, PRL, 95, 192501 (2005)

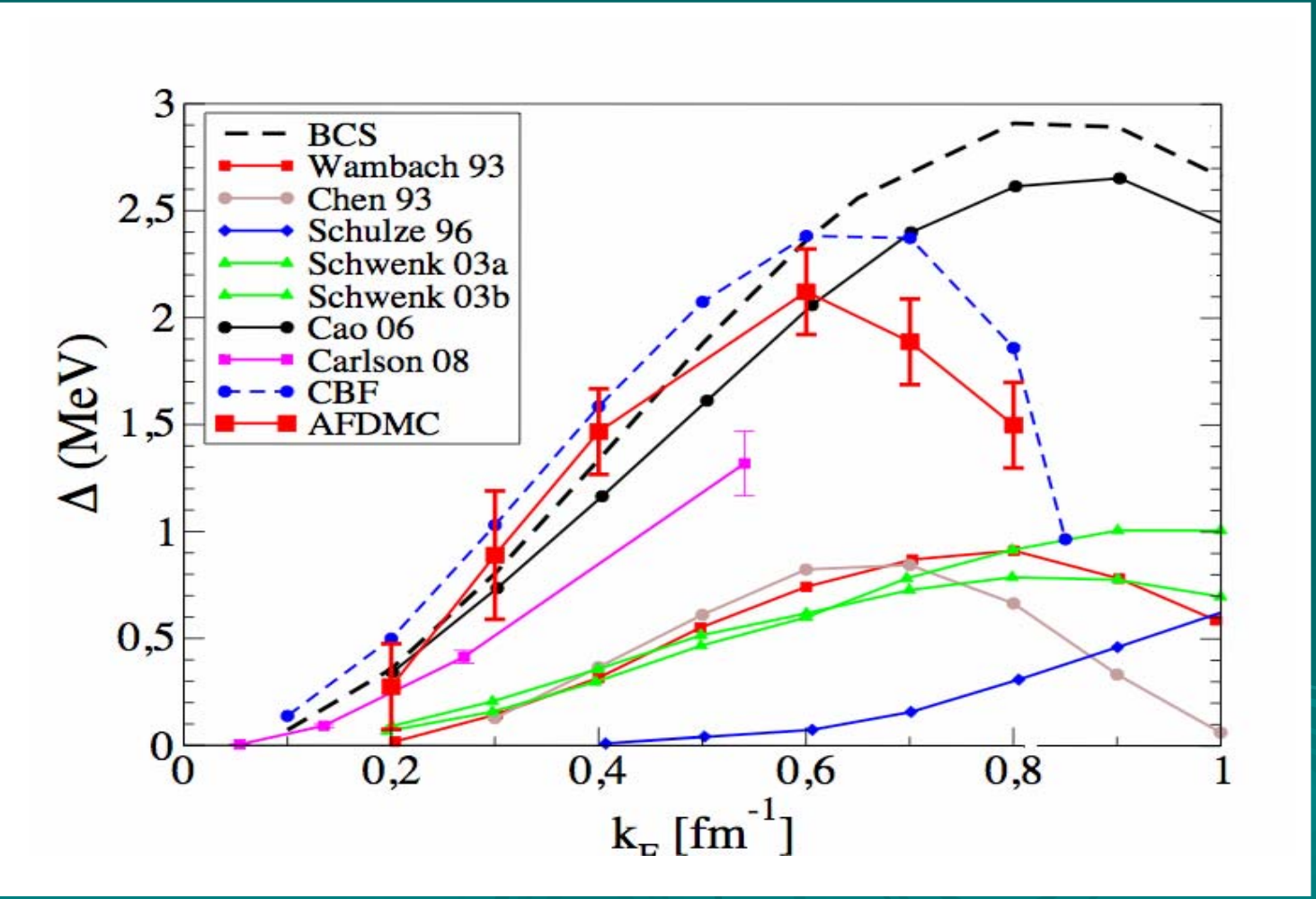
BCS versus Normal Phase

S. Gandolfi, A.Illarionov et al., 2008



GAP

S.Gandolfi, A.Illarionov et al., 2008



Nuclei

- The AFDMC has been first tested on ***light nuclei*** (^{4}He, ^{8}He) to check the consistency with other available results (few-body and GFMC calculations)
- Results for ^{16}O and ^{40}Ca are also available and are lower than VMC and CBF by 10%.

Nuclei

Wave Function

The *many-nucleon wave function* is written as the product of a ***Jastrow factor*** and an ***antisymmetric mean field wave function***:

$$\psi(\mathbf{r}_1..\mathbf{r}_N;\sigma_1..\sigma_N;\tau_1...\tau_N)=\prod_{i<j}\phi_J(r_{ij})A(\mathbf{r}_1..\mathbf{r}_N;\sigma_1..\sigma_N;\tau_1...\tau_N)$$

The functions ϕ_J in the Jastrow factor are taken as the scalar components of the FHNC/SOC correlation operator which minimizes the energy per particle of SNM at saturation density $r_0=0.16$ fm^{-1}.

Nuclei

The antisymmetric part of the wavefunction is built starting from single-particle orbitals computed with a ***HF calculation*** with ***Skyrme forces*** fitted to light nuclei. *(X. Bai and J.Hu, Phys. Rev. C 56, 1410 (1997))*

For open shell nuclei (such as ^{8}He) a wave function which is an *eigenstate of the total angular momentum* ***J*** cannot be represented in terms of a single Slater determinant → ***linear combinations of determinants are needed.***

Nuclei

AFDMC* BINDING ENERGIES OF NUCLEI (AV6')

Nucleus	E_{AFDMC} *(MeV)*	E_{GFMC} *(MeV)*
^{4}He	-27.13(10)	-26.93(1)
^{8}He	-23.6(5)	-23.6(1)
^{16}O	-100.7(4)**	------
^{40}Ca	-272(2)	------

** *VMC calculations* (S. Pieper et al.) with ***AV14***, give a binding energy of ***-83.2 MeV*** excluding contributions of terms beyond AV6. *FHNC estimates* (A. Fabrocini et al.), corrected in the same way, give a binding energy of ***-84.0 MeV***. *AFDMC* with ***AV14 truncated to AV6*** gives ***-90.8(1) MeV***.

** S. Gandolfi, F. Pederiva, SF, K.E. Schmidt, PRL, in press.*

Nuclear matter

Wave Function

The *many-nucleon wave function* for nuclear matter has a structure similar to that used for nuclei.

$$\psi(\mathbf{r}_1..\mathbf{r}_N;\sigma_1..\sigma_N;\tau_1...\tau_N)=\prod_{i<j}\phi_J(r_{ij})A(\mathbf{r}_1..\mathbf{r}_N;\sigma_1..\sigma_N;\tau_1...\tau_N)$$

The functions ϕ_J in the Jastrow factor are taken as the scalar components of the FHNC/SOC correlation operator which minimizes the energy per particle of SNM at a given density. The antisymmetric product *A* is a Slater determinant of *plane waves*.

Nuclear matter

Most simulations were performed in a ***periodic box*** containing ***28 nucleons*** (14 p and 14 n). The density was changed varying the size of the simulation box.

Particular attention must be paid to ***finite size effects***.

- At all densities we performed a summation over the first shell of periodic replicas of the simulation cell.
- Some checks against simulations with a ***larger number of nucleons (N=76,108)*** were performed at the extrema of the density interval considered.

Nuclear matter

Finite size effects

ρ/ρ_0	E/A(28) [MeV]	E/A (76) [MeV]	E/A (108) [MeV]
0.5	-7.64(3)	-7.7(1)	-7.45(2)
3.0	-10.6(1)	-10.7(6)	-10.8(1)

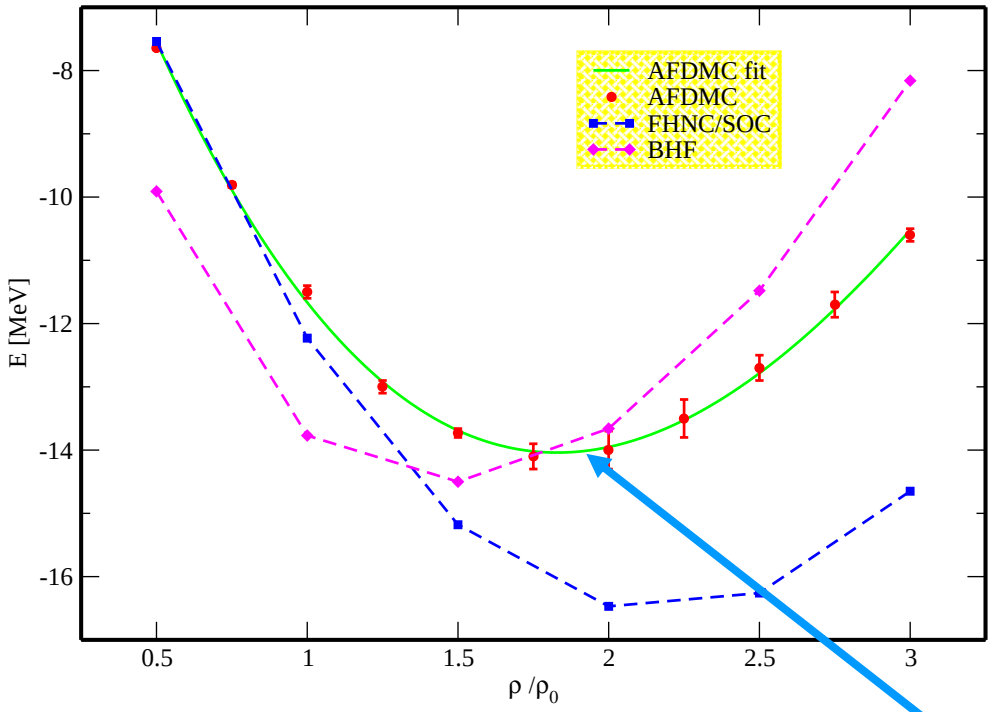
CORRECTIONS ARE LESS THAN 3%!

Nuclear matter

No three-body forces

AFDMC EOS differs from previous estimates!

We computed the energy of 28 nucleons interacting with Argonne ***AV$_8$'*** cut to ***six operators*** for several densities*, and we compare our results with those given by FHNC/SOC and BHF calculations**:



Wrong prediction of ρ_s (as expected)

** S. Gandolfi, F. Pederiva, S. Fantoni, K.E.*

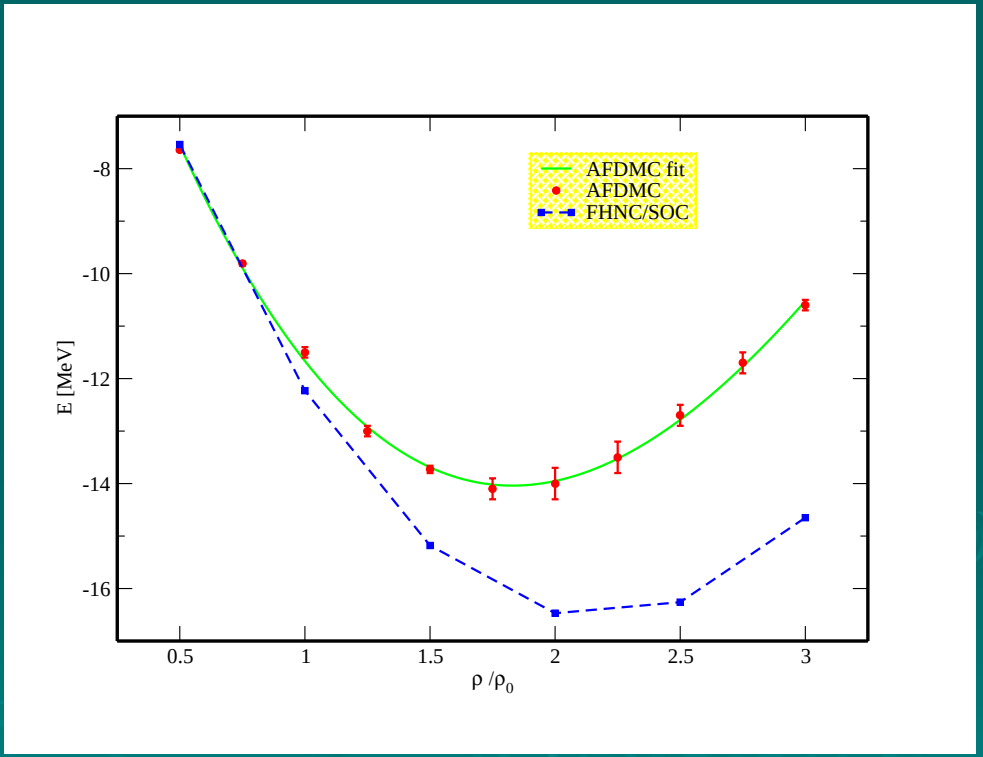
***I. Bombaci, A. Fabrocini, A. Polls, I. Vidaña, Phys. Lett. B 609, 232 (2005).*

Nuclear matter

- ***FHNC gives a larger binding energy at high density.***

FHNC/SOC contains two intrinsic approximations violating the variational principle:

1) the absence of contributions from the elementary diagrams,
2) the absence of contributions due to the non-commutativity of correlation operators entering in the variational wavefunction (SOC aproximation).



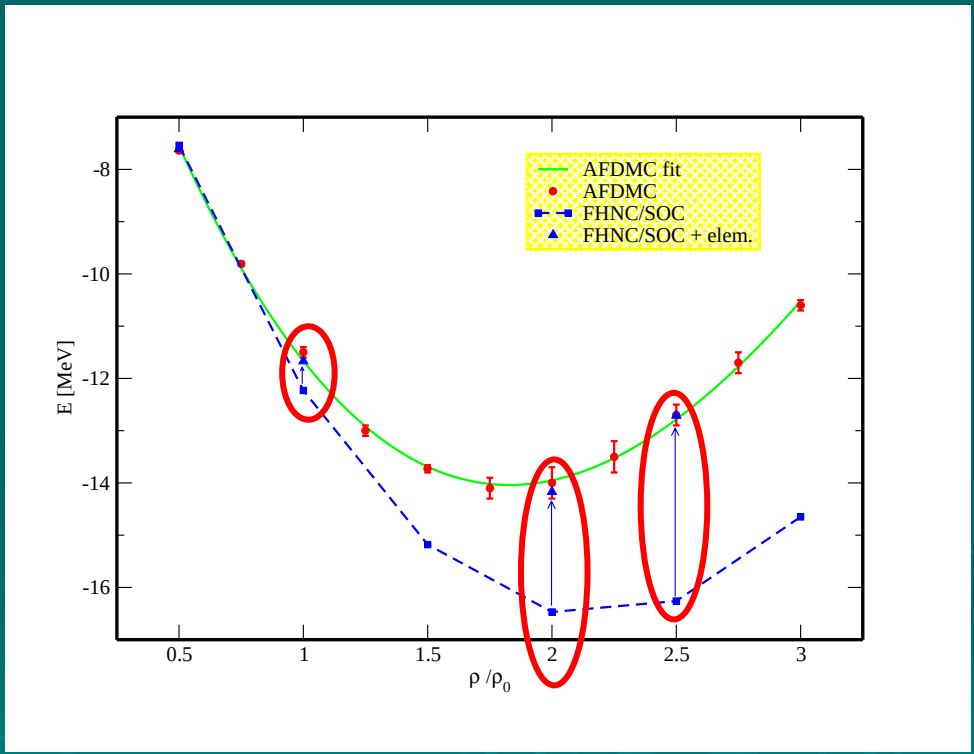
Nuclear matter

- ***Leading order corrections to FHNC/SOC***

S. Fantoni et al. computed the ***lowest order of elementary diagrams***, showing that they are **not negligible** and give an important contribution to the energy:

With the addition of this class of diagrams, ***FHNC/SOC results are much closer to the AFDMC ones.***

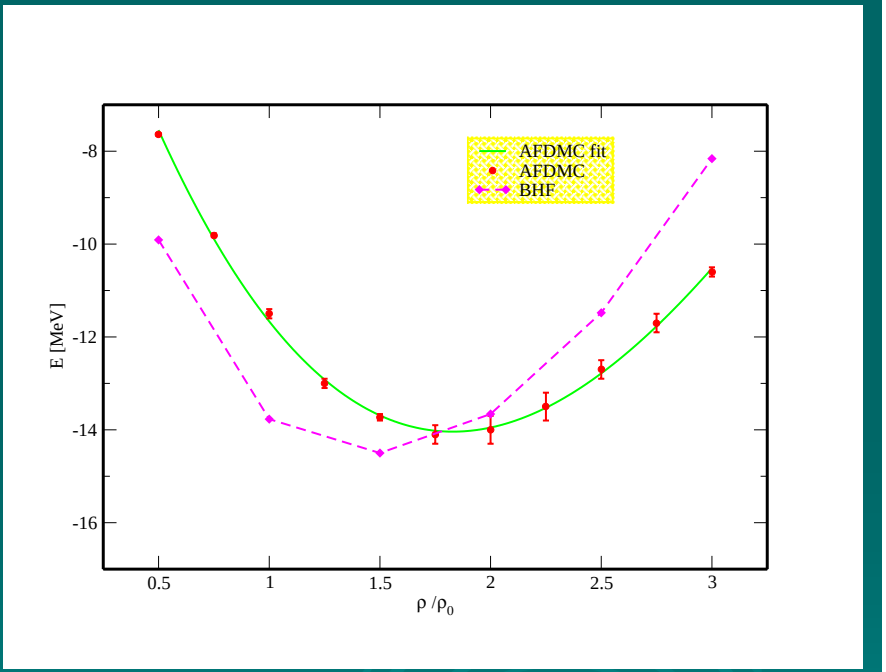
However the effect of higher order diagrams and of the SOC approximation is unknown.



Nuclear matter

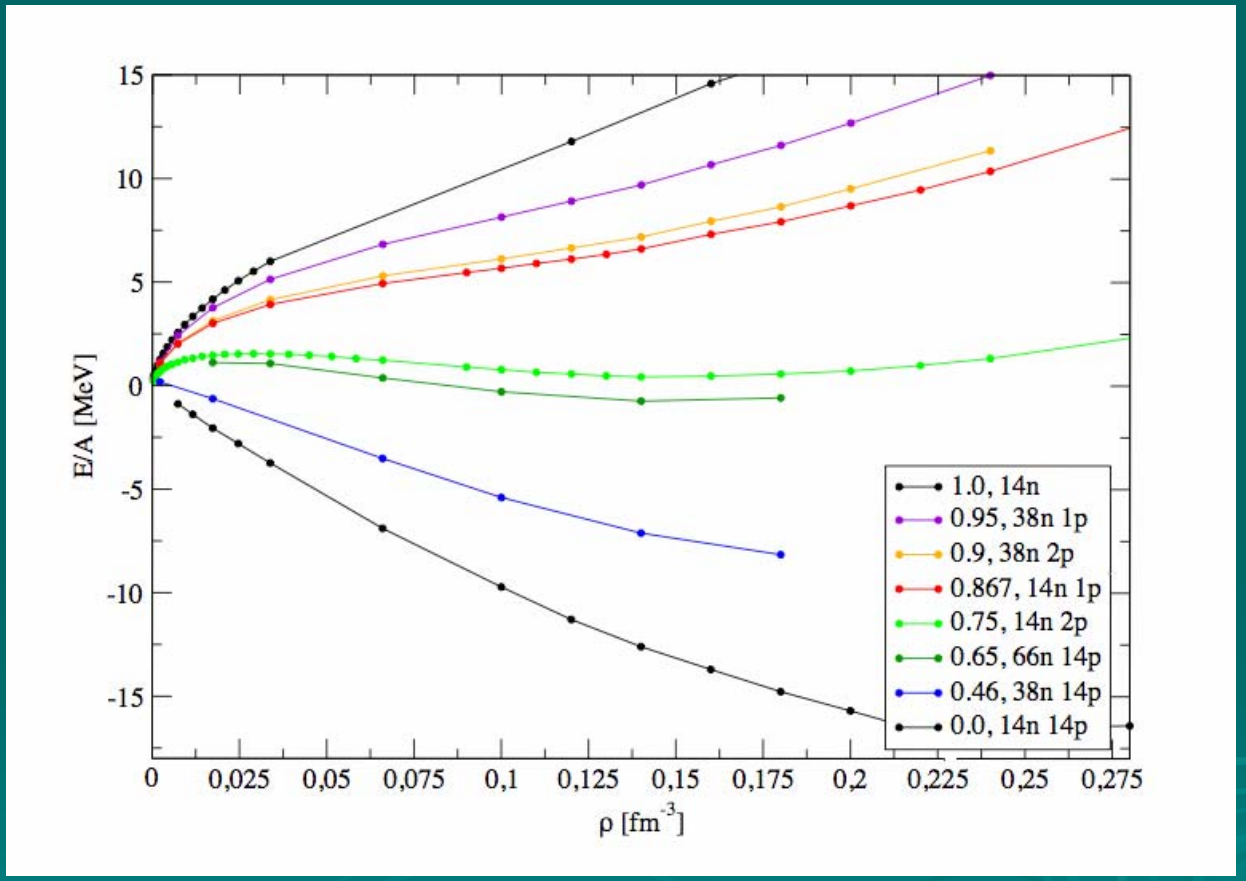
- ***BHF EOS gives a shallower binding energy***

It has been shown that for Argonne AV_{18} and AV_{14} interactions, the contribution from ***three hole-line diagrams*** in the BHF calculations add a ***positive contribution up to 3 MeV at density below ρ_0***, and ***increase the binding energy at higher densities*** *(Song et al., PRL 81, 1584 (1998)).*
Maybe for this interaction such corrections would be similar.



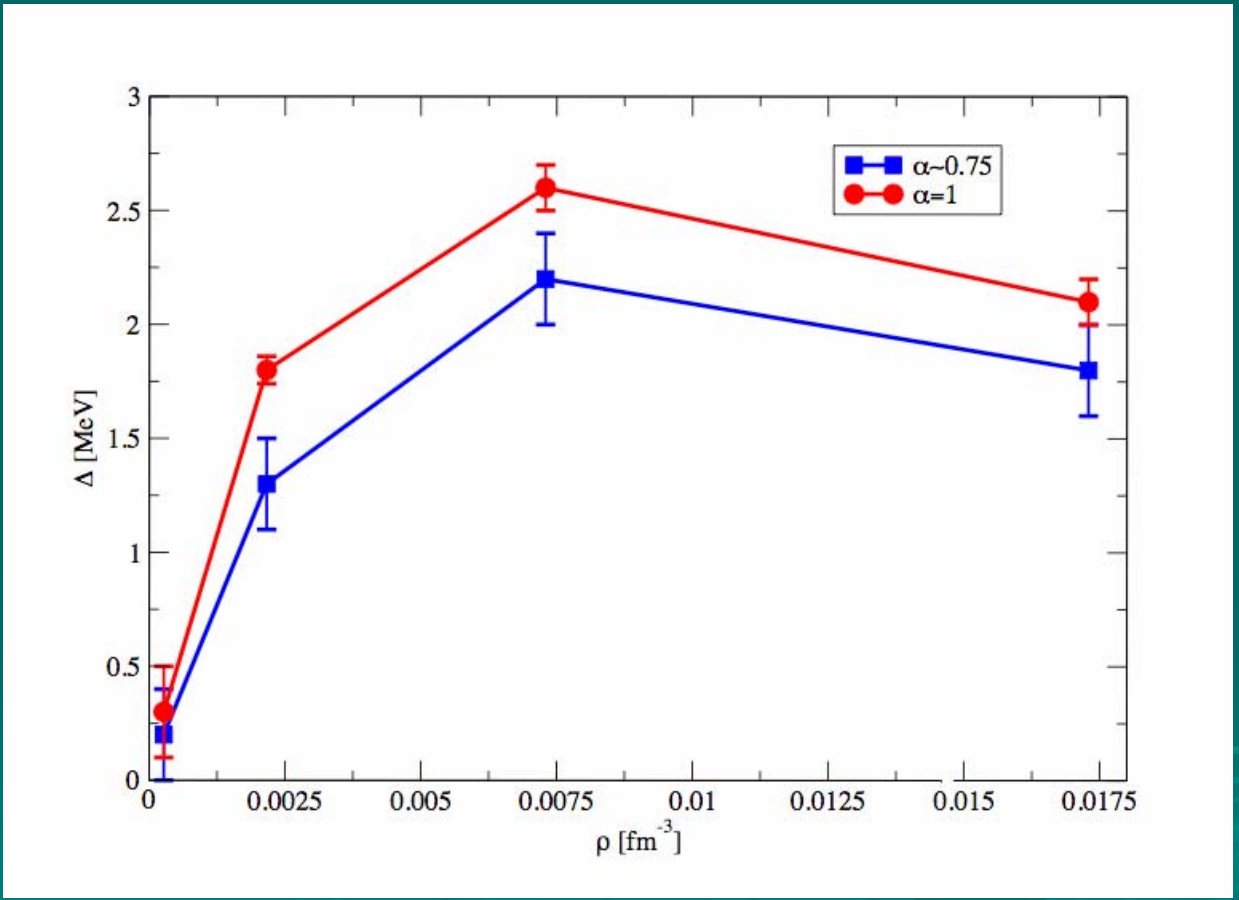
EOS asymmetric matter

A.Gandolfi et al., 2008



Gap In Asymmetric matter

S.Gandolfi, A.Illarionov, et al.., 2008



Conclusions

- AFDMC can be successfully applied to the study of nuclear matter.
- The algorithm has been successfully applied to nuclei up to ^{40}Ca (when using fixed phase approximation).
- The estimates of the EOS computed with the same potential and other methods are quite different and seem to ask for many-body interaction.
- Leading order corrections both to FHNC/SOC and BHF seem to improve the agreement.

What's next

- Add three-body forces for nuclei and nuclear matter
- Perform calculations with the full v_{18} potential
- Systematic study of nuclei (ab-initio mass formula, etc.)
- Asymmetric nuclear matter (need of twisted boundary conditions)

Three-body force

- The form of 3-body interaction is
  from the Delta resonance (Fujita-Miyazawa)
- Urbana 3-body force is obtained by integrating out the pions and the Delta assuming
  infinite masses of nucleons and Delta
- The anticommutator part is easy
  (2-body spin-isospin operators)
- The commutator part leads to 3-body spin-isospin operators. It requires double HS integrations which give large variance
- **Including explicit Delta with finite mass reduce the variance**.
- Use a fictitious Delta with $K=p^2/2m+\Delta m$ and same spin-isopsin of the nucleon. In the limit Dm going to infinity we get back Urbana IX (use of a real delta, namely 16 additional nucleon states is doable !)
- The use of a finite mass Delta include many-body forces