

Quantum Monte Carlo calculations of nuclear matter

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Outline of Talk

- Introduction
- The nuclear Hamiltonian.
- Diffusion Monte Carlo.
- Spin sampling with auxiliary field diffusion Monte Carlo method.
- Fixed Phase Approximation
- Results
- Future

Introduction

We want to be able to predict the structure of nuclei and nuclear and neutron matter.

I will talk only about ground states.

Here the Hamiltonian will be for nonrelativistic protons and neutrons interacting with a potential (mostly local).

Monte Carlo calculations need to be able to sample the nonlocal parts of the propagator.

Hamiltonian

The Hamiltonian is

$$H = \sum_i \frac{p_i^2}{2m_i} + \sum_{i < j} \sum_{p=1}^M v_p(r_{ij}) O^{(p)}(i, j) + V_3$$

- i and j label the two nucleons
- r_{ij} is the distance separating the two nucleons
- $O^{(p)}$ include central, spin, isospin, and spin orbit operators, and M is the maximum number of operators (i.e. 18 in Argonne v_{18} model).

For our calculations we use:

For purely neutron systems the Argonne v'_8 and the Urbana or Illinois three-body potentials

For nuclei and nuclear matter, we have used the Argonne v'_6 potential. We are working on including spin-orbit or three-body potentials.

The most important parts of the Urbana and Illinois three-body potentials for nuclei have a two-body spin structure and can be included easily. The other parts can sometimes be done perturbatively, but need to be done correctly to give accurate results.

The operator terms in Argonne v'_8 are

$$\begin{aligned}
 \sum_p v(r_{ij}) O_{ij}^{(p)} = & v_c(r_{ij}) + v_\tau(r_{ij}) \vec{\tau}_i \cdot \vec{\tau}_j \\
 & + v_\sigma(r_{ij}) \vec{\sigma}_i \cdot \vec{\sigma}_j + v_{\sigma\tau}(r_{ij}) \vec{\sigma}_i \cdot \vec{\sigma}_j \vec{\tau}_i \cdot \vec{\tau}_j \\
 & + v_t(r_{ij}) t_{ij} + v_{t\tau}(r_{ij}) t_{ij} \vec{\tau}_i \cdot \vec{\tau}_j \\
 & + v_{LS}(r_{ij}) (\vec{L}_i - \vec{L}_j) \cdot (\vec{S}_i + \vec{S}_j) \\
 & + v_{LS\tau}(r_{ij}) (\vec{L}_i - \vec{L}_j) \cdot (\vec{S}_i + \vec{S}_j) \vec{\tau}_i \cdot \vec{\tau}_j
 \end{aligned}$$

The central Part can be handled using standard GFMC or DMC.

The most successful method for light nuclei uses Monte Carlo for the spatial variables and complete summation over the spin-isospin states.

The number of good $S_z T_z$ spin-isospin states is

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

which can be lowered by a small factor if good T^2 states are constructed.

The exponential growth of these states limits this brute force method to ^{12}C at present.

Diffusion Monte Carlo for Central Potentials

Schrödinger equation in imaginary time (measured in units of energy⁻¹) is the diffusion equation

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

Formal solution

$$\Psi(R, t) = e^{-(H-E_T)t}\Psi(R, 0)$$
$$H\Psi_n(R) = E_n\Psi_n(R)$$
$$\Psi(R, 0) = \sum_n a_n\Psi_n(R)$$
$$\Psi(R, t) = e^{-(E_0-E_T)t}a_0\Psi_0(R) + \sum_{n\neq 0} e^{-(E_n-E_0)t}a_n\Psi_n(R)$$

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

Schematic Implementation

$$\Psi(R, t + \Delta t) = \int dR' e^{-(V(R) - E_T)\Delta t} \langle R | e^{-\frac{P^2}{2m}\Delta t} | R' \rangle \Psi(R', t)$$

- A particles (in a periodic box for matter).
- Use a short time approximation for the Green's function.
- Sample gaussian for the kinetic energy term, evaluate the diagonal potential terms as a weight.
- Use branching to control population.
- Use importance sampling to improve variance.
- For Fermions the wave function changes sign. Use fixed node or transient estimation.

Monte Carlo Spin Sampling

We want to sample the spin and isospin.

In the usual $p\uparrow, p\downarrow, n\uparrow, n\downarrow$ basis.

$R \equiv 3A$ x, y, z coordinates for the nucleons

$S \equiv A$ discrete values selecting one of $p\uparrow, p\downarrow, n\uparrow, n\downarrow$

$\Psi_T(R, S)$ = Trial wavefunction - a complex number for given R and S .

$H_{S,S'}(R)$ = the Hamiltonian

There are roughly 4^A spin-isospin states. We could sample them with low variance if we could calculate $\Psi_T(R, S)$ efficiently.

All known nontrivial trial functions require order 4^A operations to calculate either 1 or all the spin states.

We use trial functions with no spin-isospin operator correlations.

Sampling with an Auxiliary Field

We diagonalize the interaction in spinor space.

This requires $\text{Order}(A^3)$ operations – same complexity as determinant.

For A particles, the v_6 interaction can be written as

$$\begin{aligned} V &= \sum_{i < j} \left[\sum_{p=1}^6 v_p(r_{ij}) O^{(p)}(i, j) \right] = V_c + V_{nc} \\ &= V_c + \frac{1}{2} \sum_{i, \alpha, j, \beta} \sigma_{i, \alpha} A_{i, \alpha, j, \beta}^{(\sigma)} \sigma_{j, \beta} \\ &+ \frac{1}{2} \sum_{i, \alpha, j, \beta} \sigma_{i, \alpha} A_{i, \alpha, j, \beta}^{(\sigma\tau)} \sigma_{j, \beta} \vec{T}_i \cdot \vec{T}_j \\ &+ \frac{1}{2} \sum_{i, j} A_{i, j}^{(\tau)} \vec{T}_i \cdot \vec{T}_j \end{aligned}$$

- Our A matrices are zero when $i = j$ and symmetric.
- All the A matrices are real and symmetric and have real eigenvalues and eigenvectors.
- The eigenvectors and eigenvalues are defined by

$$\sum_{j,\beta} A_{i,\alpha,j,\beta}^{(\sigma)} \vec{\psi}_n^\sigma(j) \cdot \hat{x}_\beta = \lambda_n^{(\sigma)} \vec{\psi}_n^\sigma(i) \cdot \hat{x}_\alpha$$

The matrices can be written in terms of their eigenvectors and eigenvalues to give the noncentral potential

$$\begin{aligned} V_{nc} &= \frac{1}{2} \sum_{i,j,n} \vec{\sigma}_i \cdot \vec{\psi}_n^{(\sigma)}(i) \lambda_n^{(\sigma)} \vec{\psi}_n^{(\sigma)}(j) \cdot \vec{\sigma}_j \\ &+ \frac{1}{2} \sum_{i,j,n} \vec{\sigma}_i \cdot \vec{\psi}_n^{(\sigma\tau)}(i) \lambda_n^{(\sigma\tau)} \vec{\psi}_n^{(\sigma\tau)}(j) \cdot \vec{\sigma}_j \vec{\tau}_i \cdot \vec{\tau}_j \\ &+ \frac{1}{2} \sum_{i,j,n} \vec{\tau}_i \cdot \vec{\tau}_j \psi_n^{(\tau)}(i) \lambda_n^{(\tau)} \psi_n^{(\tau)}(j) \end{aligned}$$

We want the squares of operators so we write

$$\begin{aligned}
 V_{nc} &= \frac{1}{2} \sum_{n=1}^{3A} (O_n^{(\sigma)})^2 \lambda_n^{(\sigma)} \\
 &+ \frac{1}{2} \sum_{\alpha=1}^3 \sum_{n=1}^{3A} (O_{n\alpha}^{(\sigma\tau)})^2 \lambda_n^{(\sigma\tau)} \\
 &+ \frac{1}{2} \sum_{\alpha=1}^3 \sum_{n=1}^A (O_{n\alpha}^{(\tau)})^2 \lambda_n^{(\tau)}
 \end{aligned}$$

with

$$O_n^{(\sigma)} = \sum_i \vec{\sigma}_i \cdot \vec{\psi}_n^{(\sigma)}(i)$$

$$O_{n\alpha}^{(\sigma\tau)} = \sum_i \tau_{i\alpha} \vec{\sigma}_i \cdot \vec{\psi}_n^{(\sigma\tau)}(i)$$

$$O_{n\alpha}^{(\tau)} = \sum_i \tau_{i\alpha} \psi_n^{(\tau)}(i)$$

- The Hubbard-Stratonovich transformation is

$$e^{-\frac{1}{2}\lambda_n O_n^2 \Delta t} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-\frac{1}{2}x^2 + x\sqrt{-\lambda_n \Delta t} O_n}$$

- Our O_n don't commute, so we need to keep the time steps small so that the commutator terms can be ignored. Each of the O_n is a sum of 1-body operators as required above.
- We require $3A$ Hubbard-Stratonovich variables for the σ terms, $9A$ variables for the $\sigma\tau$ terms, and $3A$ variables for the τ terms. Each time step requires the diagonalization of two $3A$ by $3A$ matrices and one A by A matrix.
- Many other breakups are possible.

Constrained Path

- We still have the usual fermi sign problem, in this case the overlap of our walkers with the trial function will be complex.
- We constrain the path so that the walker has the same phase as the trial function, and deform the path of the auxiliary field integration so that the auxiliary variables are complex[†].
- For spin independent potentials this reduces to the fixed-node or fixed phase approximation.
- There is a variational principle for the mixed energy but not an upper bound principle. Expectation values of H have an upper bound principle but are not implemented here.

[†] S. Zhang and H. Krakauer, *Quantum Monte Carlo method using phase-free random walks with Slater determinants*, Phys. Rev. Lett. **90**, 136401 (2003).

Results for neutron systems

- Neutron Matter Equation of State[†].
- Neutron Matter Spin Susceptibility[‡].
- Model Neutron Drops (Unambiguous comparison to GFMC)[§].
- Even odd energy gaps using Pfaffian trial functions for 1S_0 BCS pairing in low density neutron matter[¶].

[†] S. Gandolfi, et al., Quantum Monte Carlo calculation of the equation of state of neutron matter , in preparation. M. Bouadani, et al., Pion condensation in high density neutron matter, in preparation. A. Sarsa, S. Fantoni, K. E. Schmidt and F. Pederiva, *Neutron matter at zero temperature with auxiliary field diffusion Monte Carlo method*, Phys. Rev. C **68**, 024308 (2003).

[‡] S. Fantoni, A. Sarsa, K.E. Schmidt, *Spin Susceptibility of Neutron Matter at Zero Temperature*, Phys. Rev. Lett. **87**, 181101 (2001).

[§] S. Gandolfi, K.E. Schmidt, F. Pederiva, and S. Fantoni, Three nucleon interaction role in neutron drops, in preparation. F. Pederiva, A. Sarsa, K. E. Schmidt and S. Fantoni, Auxiliary field diffusion Monte Carlo calculation of ground state properties of neutron drops, Nucl. Phys. A **742**, 255 (2004).

[¶]A. Fabrocini, S. Fantoni, A. Yu Illarionov, and K.E. Schmidt, 1S_0 superfluid phase transition in neutron matter with realistic nuclear potentials and modern many-body theories, Phys. Rev. Lett. **95**, 192501 (2005); and S. Gandolfi, F. Pederiva, A. Illarionov, S. Fantoni, and K.E. Schmidt, in press (2008).

Results for neutron and proton systems

- Symmetric nuclear matter.[†]
- Selected nuclei.[‡]
- Asymmetric matter – some preliminary results.

[†]S. Gandolfi, F. Pederiva, S. Fantoni, and K. E. Schmidt Quantum Monte Carlo Calculations of Symmetric Nuclear Matter Phys. Rev. Lett. **98**, 102503 (2007).

[‡] S. Gandolfi, F. Pederiva, S. Fantoni, and K. E. Schmidt, Auxiliary Field Diffusion Monte Carlo Calculation of Nuclei with A40 with Tensor Interactions, Phys. Rev. Lett. **99**, 022507 (2007).

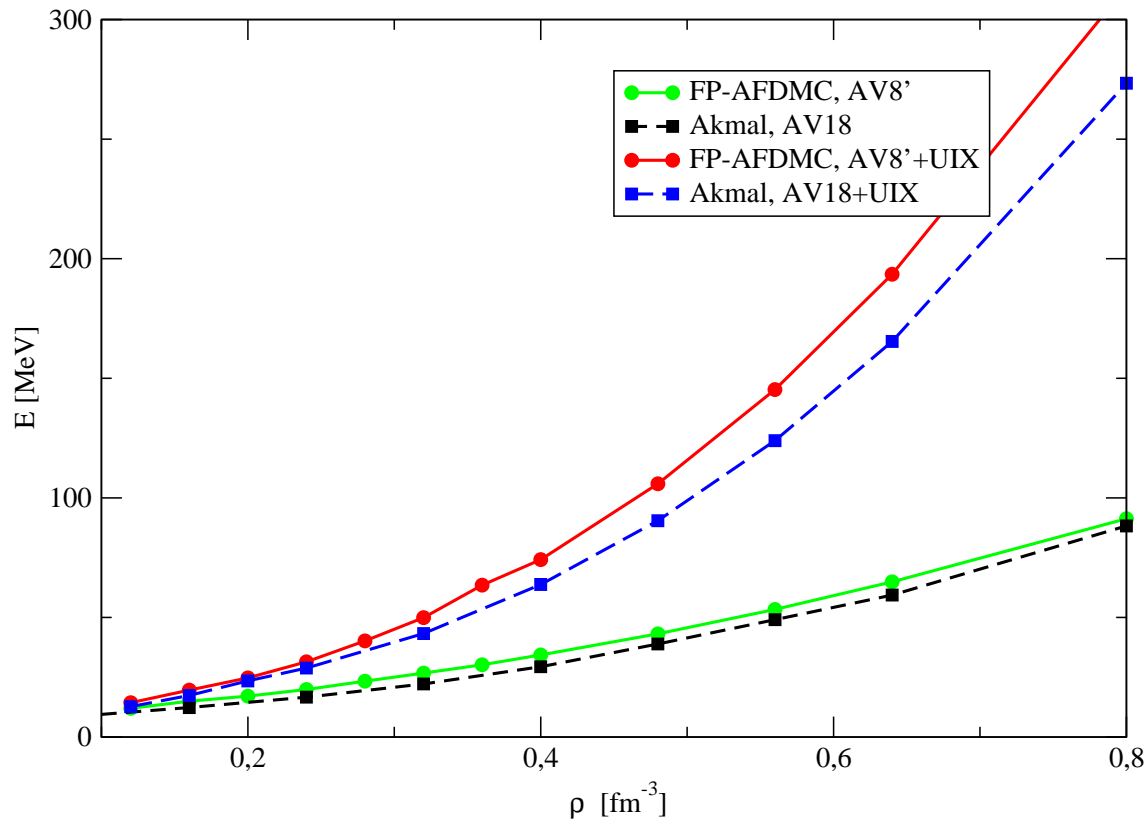
GFMC Model neutron drop comparison

Table 1: Ground state AFDMC energies of ${}^8n(0^+)$, ${}^7n(\frac{1}{2}^+)$ and ${}^7n(\frac{3}{2}^+)$ droplets for $V_0 = 20\text{MeV}$ and the AU8' and AU6' interactions. The cluster variational Monte Carlo (CVMC) and GFMC results[†] for the AU8' and the full AU18 (Argonne v_{18} plus Urbana IX) are also reported for comparison. The last column reports the spin-orbit splittings (SOS) in MeV of 7n , given by the energy difference between the ${}^7n(\frac{3}{2}^+)$ and ${}^7n(\frac{1}{2}^+)$ states.

	${}^8n(0^+)$	${}^7n(\frac{1}{2}^+)$	${}^7n(\frac{3}{2}^+)$	SOS
GFMC(AU18)	-37.8(1)	-33.2(1)	-31.7(1)	1.5(2)
CVMC(AU18)	-35.5(1)	-31.2(1)	-29.7(1)	1.5(2)
GFMC(AU8')	-38.3(1)	-34.0(1)	-32.4(1)	1.6(2)
AFDMC(AU8')	-37.55(2)	-33.06(3)	-31.51(2)	1.55(5)

[†] S. C. Pieper, V. R. Pandharipande, R. B. Wiringa, and J. Carlson, *Realistic models of pion-exchange three-nucleon interactions*, Phys. Rev. C **64**, 14001 (2001).

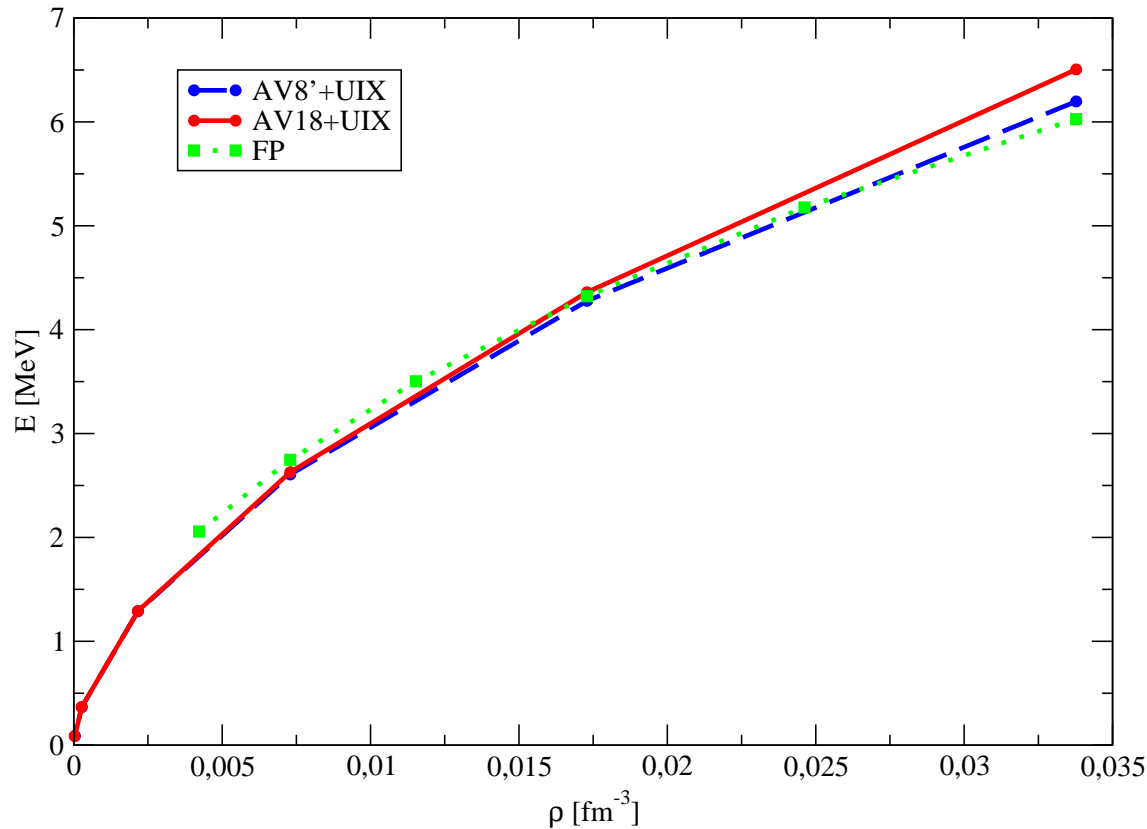
Neutron matter equation of state



Akmal refers to the FHNC calculation[†]

[†] A. Akmal, V.R. Pandharipande, and D.G. Ravenhall, Equation of state of nucleon matter and neutron star structure, Phys. Rev. C **58** 1804 (1998).

Low density neutron matter with Argonne v_{18}



FP is the calculation of Friedman and Pandharipande (not v_{18} , but the low energy channels are not very different).[†]

[†] B. Friedman and V.R. Pandharipande, Hot and cold, nuclear and neutron matter, Nucl. Phys. A **361**, 502 (1981).

Superfluid wave functions

We use a BCS form used here which is the standard BCS form projected onto N particles.

For a bulk system of spin singlet pairs,

$$|BCS\rangle = \prod_{\vec{k}} \left[u_k + v_k c_{\vec{k}\uparrow}^+ c_{-\vec{k}\downarrow}^+ \right] |0\rangle$$
$$\phi(\vec{r}_1, s_1; \vec{r}_2, s_2) \propto \sum_{\vec{k}} \frac{v_k}{u_k} \cos(\vec{k} \cdot [\vec{r}_1 - \vec{r}_2]) [\langle s_1 s_2 | \uparrow\downarrow \rangle - \langle s_1 s_2 | \downarrow\uparrow \rangle]$$

In general

$$|BCS\rangle = \prod_n [u_n + v_n c_n^+ c_{n'}^+] |0\rangle$$
$$\phi(\vec{r}_1, s_1; \vec{r}_2, s_2) \propto \sum_n \frac{v_n}{u_n} [\psi_n(\vec{r}_1, s_1) \psi_{n'}(\vec{r}_2, s_2) - \psi_n(\vec{r}_2, s_2) \psi_{n'}(\vec{r}_1, s_1)]$$

Combinations of paired and unpaired orbitals

A general state with n paired and o unpaired orbitals for a total of $N = 2n + o$ particles can be written as

$$\mathcal{A}[\phi_{12}\phi_{34}\dots\phi_{2n-1,2n}\dots\psi_1(2n+1)\dots\psi_o(N)]$$

which is the Pfaffian of the $(N + o) \times (N + o)$ matrix

$$\begin{pmatrix} 0 & \phi_{12} & \phi_{13} & \dots & \phi_{1N} & \psi_1(1) & \dots & \psi_o(1) \\ -\phi_{12} & 0 & \phi_{23} & \dots & \phi_{2N} & \psi_1(2) & \dots & \psi_o(2) \\ -\phi_{13} & \phi_{23} & 0 & \dots & \phi_{3N} & \psi_1(3) & \dots & \psi_o(3) \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ -\phi_{1N} & -\phi_{2N} & -\phi_{3N} & \dots & 0 & \psi_1(N) & \dots & \psi_o(N) \\ -\psi_1(1) & -\psi_1(2) & -\psi_1(3) & \dots & -\psi_1(N) & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ -\psi_o(1) & -\psi_o(2) & -\psi_o(3) & \dots & -\psi_o(N) & 0 & \dots & 0 \end{pmatrix},$$

where the lower $o \times o$ section is all zeroes.

Spin singlet pairing reduces to a determinant. Calculations of Pfaffians – $O(N^3)$ operations[†]

[†] M. Bajdich, L. Mitas, L. K. Wagner and K. E. Schmidt, *Pfaffian Pairing and backflow wave functions for electronic-Structure Quantum Monte Carlo methods*, Phys. Rev. B" **77**, 115112 (2008).

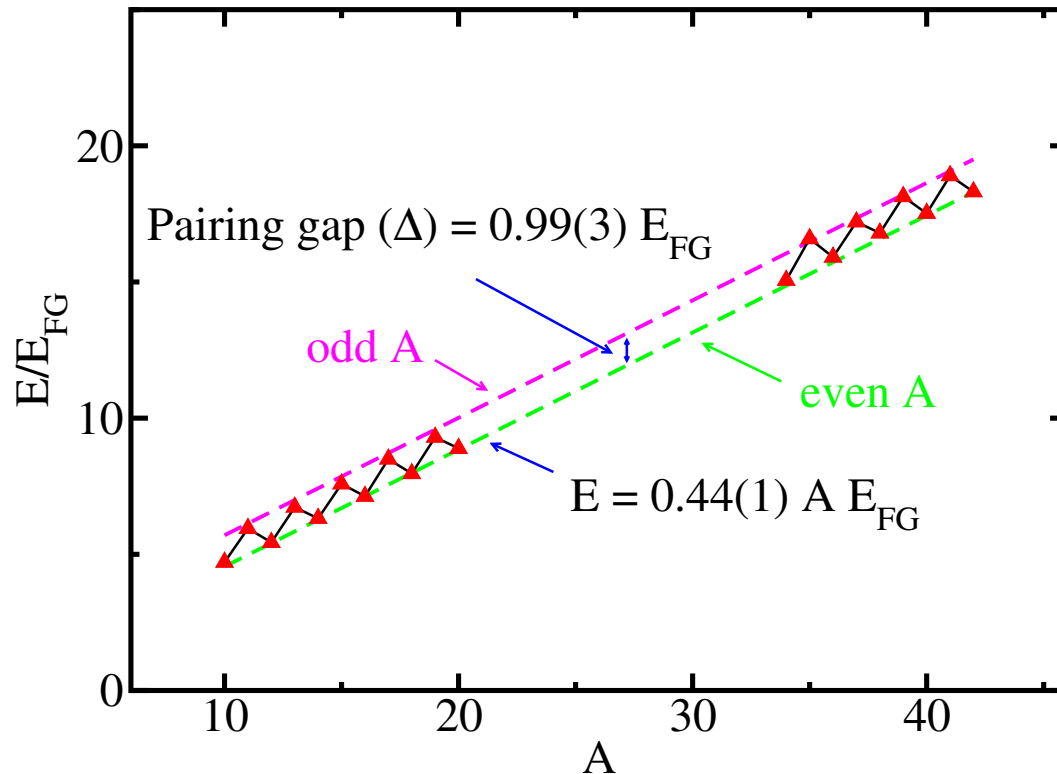
Central Spin Singlet Application

Dilute \equiv range R of the interaction \ll than interparticle spacing r_0 , or $k_F R \ll 1$, $\rho = \frac{3}{4\pi r_0^3} = \frac{k_F^3}{3\pi^2}$

If the scattering length a is large – short range interactions can strongly modify the dilute gas properties, $k_F |a| \gg 1$.

Low density neutron matter (in inner crust of neutron stars) $R \sim 2$ fm, $a = -18$ fm.

Energy and even-odd energy gap for $a = -\infty$ [†]



Energy as a function of particle number A .

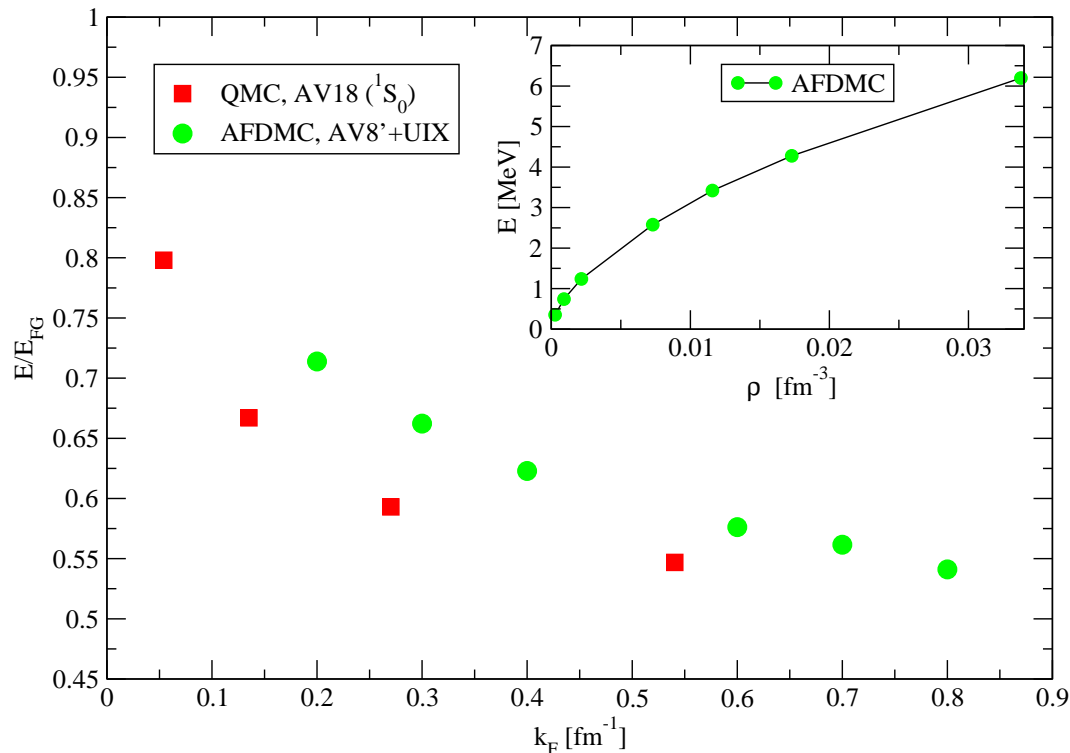
Slater determinant nodes give an energy of $E/A = 0.54E_{FG}$.

[†]J. Carlson, S-Y Chang, V.R. Pandharipande, and K.E. Schmidt, "Superfluid Fermi Gases with Large Scattering Length", Phys. Rev. Lett. **91**, 050401 (2003).

Neutron Matter pairing

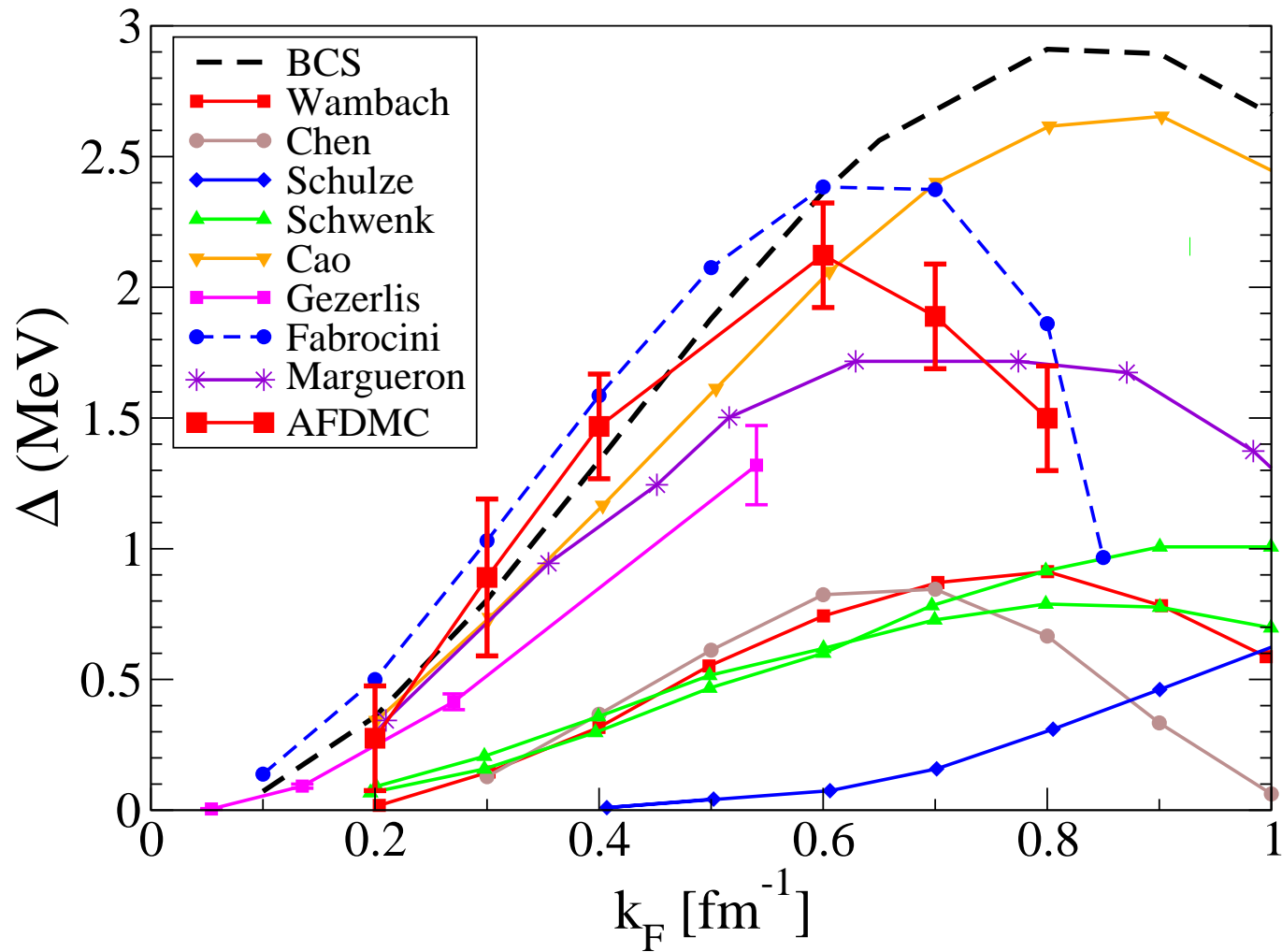
We begin with Fermi-hypernetted chain correlated basis function method to produce the trial wave function for the constraint.

Even though the dominant low density pairing is spin singlet, since the particles' spin can be flipped by the potential, the Pfaffian is needed.



Calculated BCS versus normal equation of state

Neutron matter energy gaps



Calculated energies gap (AFDMC) compared to other calculations.

Spin Susceptibility

ρ/ρ_0	Reid [†]	Reid6 [‡]	AU6'	AU8'	Reid6
0.75	0.45	0.53	0.40(1)		
1.25	0.42	0.50	0.37(1)	0.39(1)	0.36(1)
2.0	0.39	0.47	0.33(1)	0.35(1)	
2.5	0.38	0.44	0.30(1)		

Spin susceptibility ratio χ/χ_F of neutron matter. The AFDMC results for the interactions AU6', AU8' and Reid6 are compared with those obtained from the Landau parameters calculated from FHNC and CBF theories. The statistical error is given in parentheses.

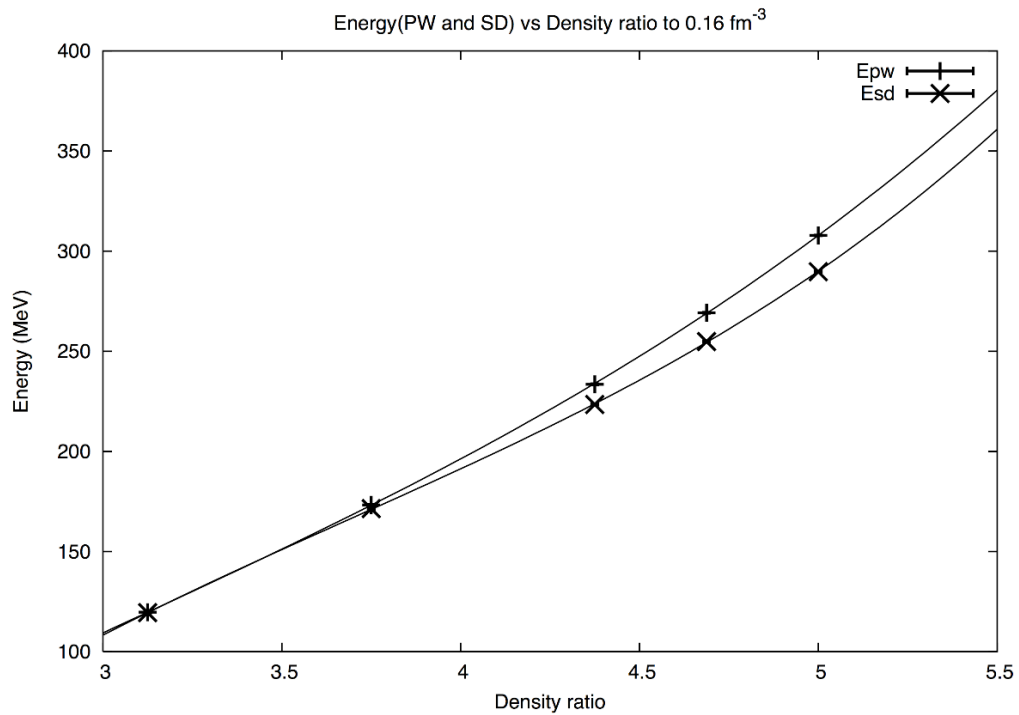
[†] Brueckner calculations by S. O. Bäckmann and C. G. Källman, Phys. Lett. B **43** (1973) 263.

[‡] CBF calculations by A. D. Jackson, E. Krotscheck, D. E. Meltzer and R. A. Smith, Nucl. Phys. A **386** (1992) 125.

Pion Condensate in neutron matter

- It has been conjectured that a “pion condensate” occurs in neutron stars
- This refers to a spin-density wave in neutron matter at high densities.
- The $\vec{\sigma} \cdot \vec{\nabla} \pi$ coupling to the pion field indicates that such a wave would be accompanied by a pion field with a nonzero ground-state expectation – sort of a condensate.

Pion Condensate Results



PW = Plane wave model state

SD = Spin density wave model state

He Isotopes

${}^4\text{He}$

AFDMC v'_6 -27.13(10) MeV

Hyperspherical v'_6 -26.93(1) MeV[†]

GFMC v'_6 -26.93(1) MeV [-26.23(1) -0.7 MeV Coulomb][‡]

Expt -28.296 MeV

${}^8\text{He}$

AFDMC v'_6 -23.6(5) MeV (Unstable to breakup into ${}^4\text{He}+2n$)

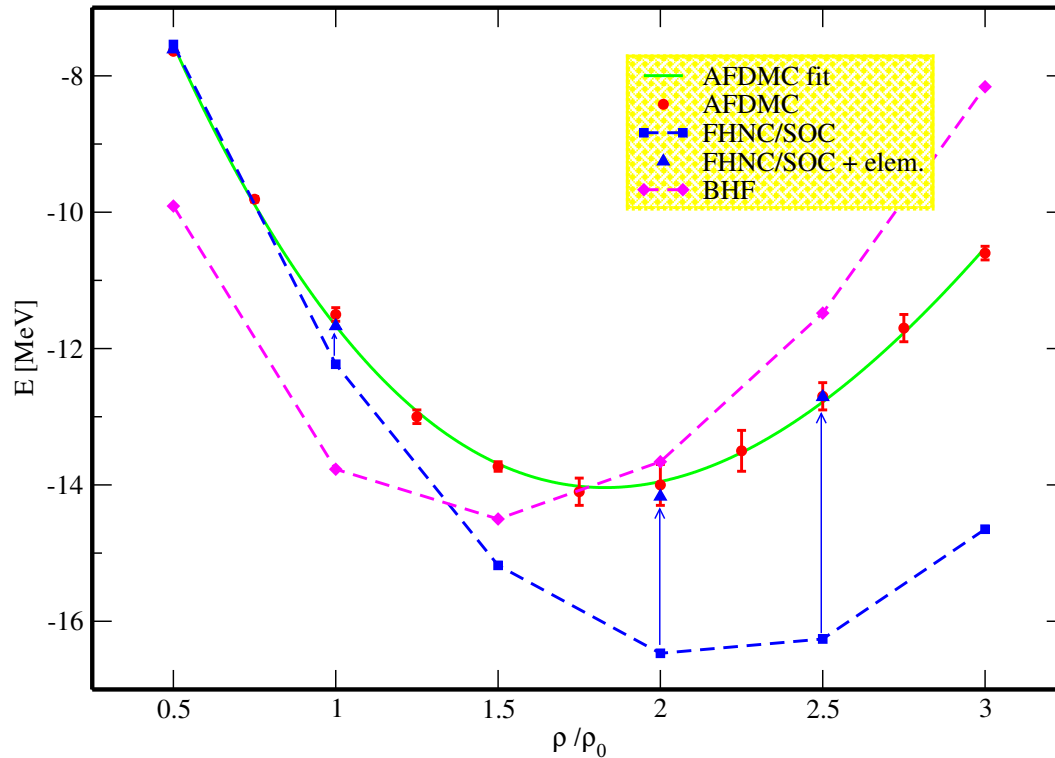
GFMC v'_6 -23.55(8) MeV [-22.85(8) -0.7 MeV Coulomb]

Expt -31.408 MeV

[†] G. Orlandini, private communication

[‡] R.B. Wiringa and S.C. Pieper, *Evolution of Nuclear Spectra with Nuclear Forces*, Phys. Rev. Lett. **89**, 182501 (2002).

Nuclear matter Energy, 28 particles, v'_8 truncated to v_6



Dashed lines correspond to calculations performed with other methods[†] (blue line with squares: FHNC/SOC; magenta with diamonds: BHF). Blue triangles are FHNC/SOC results corrected with elementary diagrams.

[†] I. Bombaci, A. Fabrocini, A. Polls, I. Vidaña, *Spin-orbit tensor interactions in homogeneous matter of nucleons: accuracy of modern many-body theories*, Phys. Lett. B, **609**, 232 (2005).

The AFDMC equation of state is fit to

$$\frac{E}{A} = \frac{E_0}{A} + \alpha(x - \bar{x})^2 + \beta(x - \bar{x})^3,$$

$$x = \rho/\rho_0 \quad \rho_0 = 0.16 \text{ fm}^{-3}.$$

$$E_0/A = -14.04(4) \text{ MeV}$$

$$\alpha = 3.09(6) \text{ MeV}$$

$$\beta = -0.44(8) \text{ MeV}$$

$$\bar{x} = 1.83(1)$$

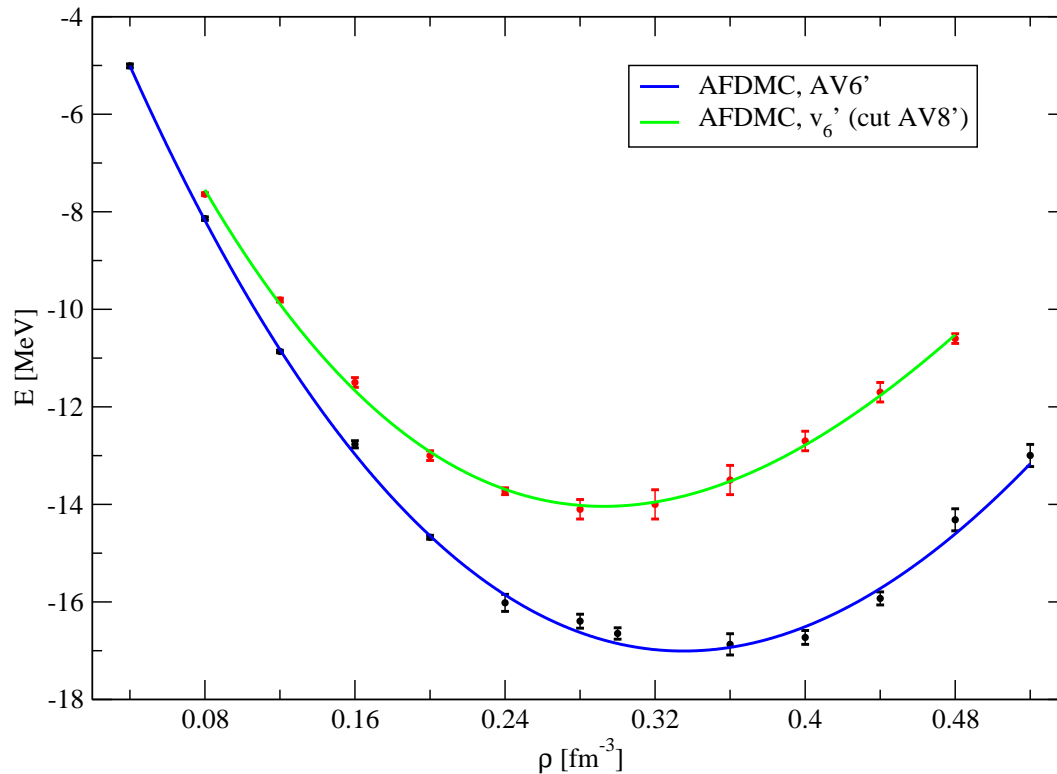
The compressibility

$$K = 9\bar{x}^2 \left(\partial^2 (E/A) / \partial x^2 \right)_{\bar{x}} \text{ at saturation density } \bar{x} \text{ is } \sim 190 \text{ MeV}.$$

Results with 76 and 108 particles are within 3 percent of those for 28 particles.

Nuclear matter with Argonne v'_6

Symmetric nuclear matter.

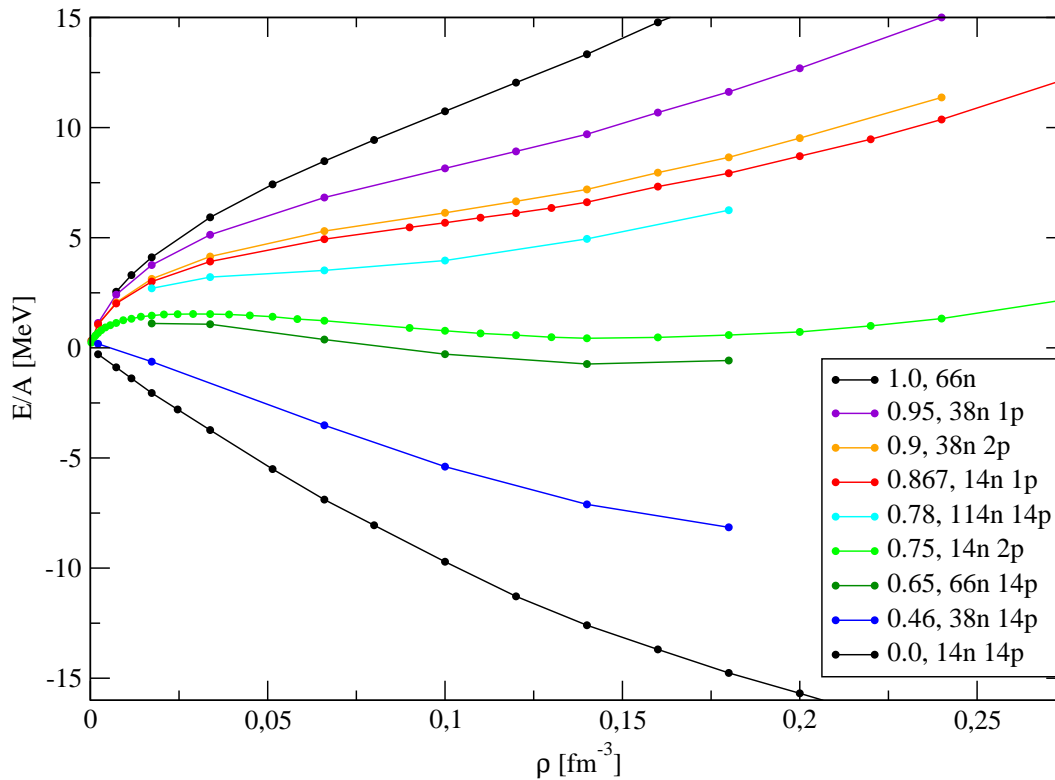


Comparison between Argonne v'_8 truncated to v_6 and Argonne v'_6 .

Asymmetric matter – some initial results

It's easy to calculate with different numbers of neutrons and protons.

Removing size dependence is important.



These are for Argonne v'_6 .

Conclusions and Future

- The auxiliary field Diffusion Monte Carlo calculations can give accurate results for nuclei, neutron and nuclear matter.
- They have polynomial scaling with system size
- The three-body and spin-orbit potentials need to be included for the neutron-proton case.
- Asymmetric matter is straightforward, but size dependence needs to be addressed.
- Physics of neutron rich nuclei can be studied – these are difficult to produce in laboratories, but important for R-process reactions.
- Temperature > 0 is possible.