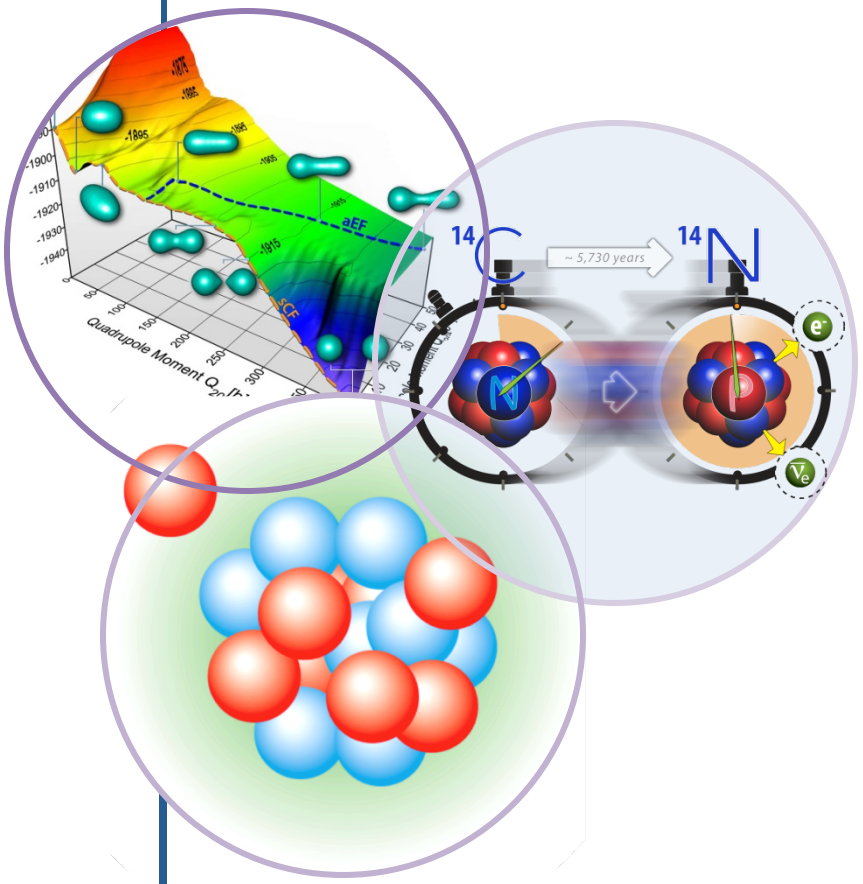
Infinite nucleonic matter from coupled-cluster theory

Gaute Hagen (ORNL)



Lecture 1-2, TALENT school

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Coupled-cluster computations of atomic nuclei

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Abstract. In the past decade, coupled-cluster theory has seen a renaissance in nuclear physics, with computations of neutron-rich and medium-mass nuclei. The method is efficient for nuclei with product-state references, and it describes many aspects of weakly bound and unbound nuclei. This report reviews the technical and conceptual developments of this method in nuclear physics, and the results of coupled-cluster calculations for nucleonic matter, and for exotic isotopes of helium, oxygen, calcium, and some of their neighbors.

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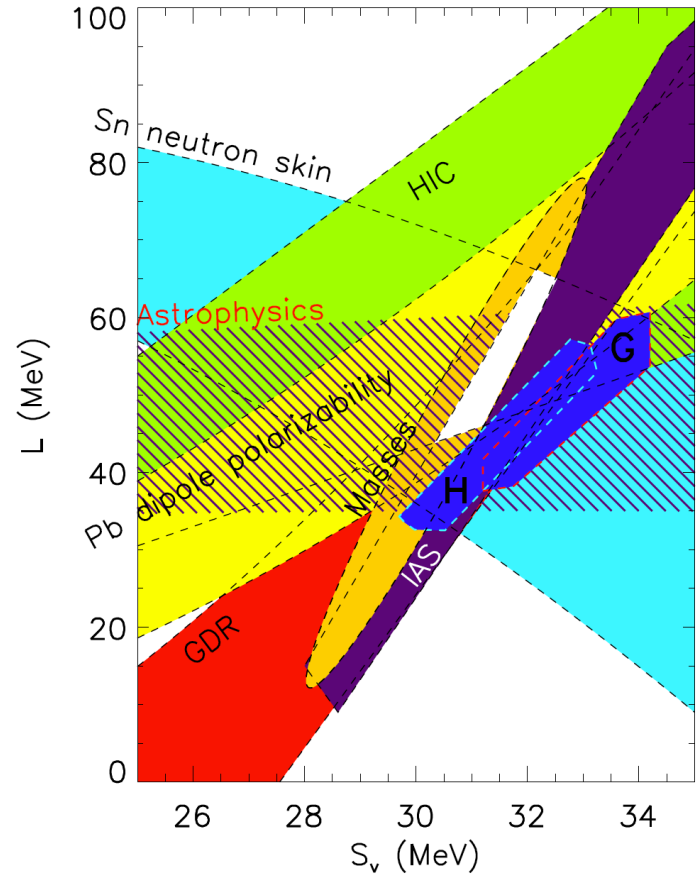
Outline

- Why study infinite nucleonic matter?
- Infinite nucleonic matter using periodic boundary conditions
- Setting up single-particle basis
- The Minnesota potential and computation of matrix elements in plane-wave basis
- Hartree-Fock for infinite matter using periodic boundary conditions
- Finite size effects and twist-averaging
- Going beyond mean-field
  - Many-body perturbation theory
  - Coupled-cluster in ladder approximation
  - Coupled-cluster doubles (CCD) approximation
- Recent applications of CCD to infinite nucleonic matter with chiral nucleon-nucleon and three-nucleon interactions

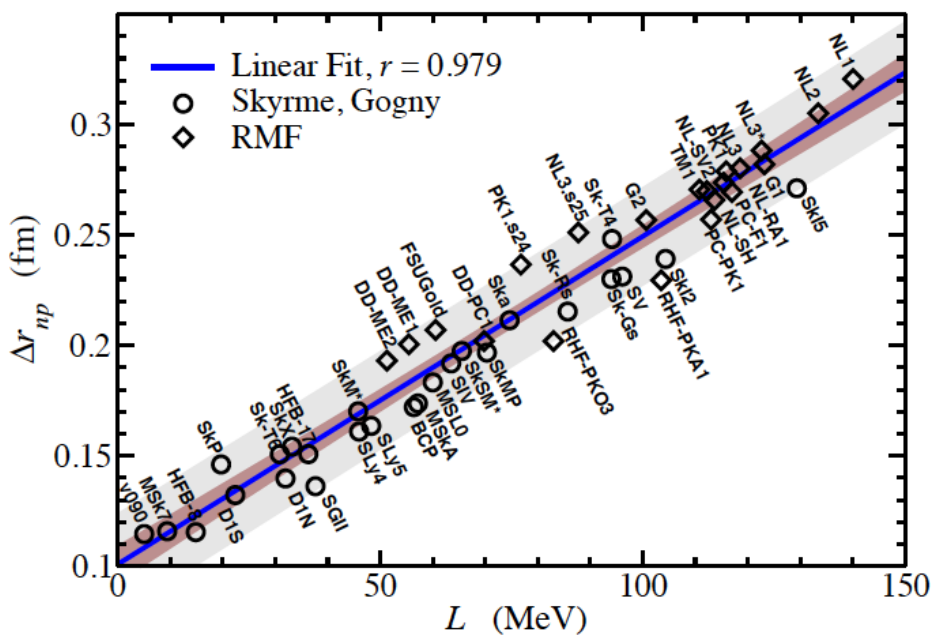
Why infinite nucleonic matter?

- Determines properties of supernova explosions and of neutron stars
- Equation of state links neutron stars to neutron radii in atomic nuclei
- The symmetry energy of nucleonic matter is related to the neutron skin



Lattimer & Steiner, EPJA 50 (2014) 40

X. Viñas et al, Eur. Phys. J. A 50, 27 (2014)



- The incompressibility is probed in giant dipole excitations in nuclei
- The nuclear matter saturation point from first principles is a challenge

Nucleonic matter from periodic boundary conditions

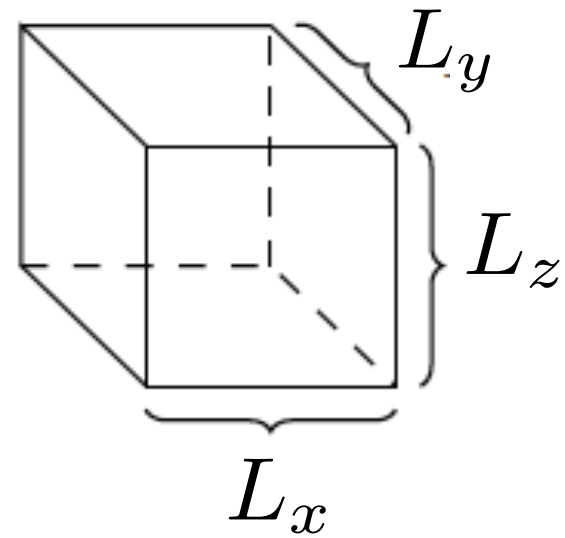
- Standard way to solve the infinite matter problem is to solve integral equations in relative center-of-mass frame using a partial wave expansion (e.g. Brueckner-Bethe-Goldstone theory)
  - Difficult to treat particle-hole correlations
  - Easy to extrapolate to thermodynamic limit

- Here we will focus on solving the infinite matter problem using periodic boundary conditions (PBC)
  - Straightforward to include all classes of correlations (e.g. particle-hole)
  - No partial wave expansion makes it easier to code
  - More difficult to extrapolate to thermodynamic limit
  - Finite size effects often non-negligible (can be minimized using twist-averaged periodic boundary conditions)
  - Due to momentum conservation there are no singles excitations

Periodic boundary conditions (PBC) in 3D

Schrodinger equation for plane waves in a cubic box

$$\frac{-\hbar}{2m}\nabla^2\phi(\mathbf{x}) = \varepsilon\phi(\mathbf{x})$$



Periodic boundary conditions gives:

$$\phi(x,y,z) = \phi(x+L_x,y,z)$$
$$\phi(x,y,z) = \phi(x,y+L_y,z)$$
$$\phi(x,y,z) = \phi(x,y,z+L_z)$$

Assume box of equal sides: $L = L_x = L_y = L_z$

Thies yields normalized plane wave solutions with discrete momenta:

$$\phi_n(\mathbf{x}) = \frac{1}{\sqrt{V}}e^{i\mathbf{k}_n\mathbf{x}} \qquad k_{n_i} = \frac{2\pi n_i}{L}$$

$$n_i = 0, \pm 1, \pm 2, \ldots$$

Periodic boundary conditions in 3D

- The energy eigenvalues (ordered)

$$\varepsilon_n = \frac{\hbar^2}{2m}\left(k_{n_x}^2 + k_{n_y}^2 + k_{n_z}^2\right)$$

yield closed shell "Fermi" spheres:

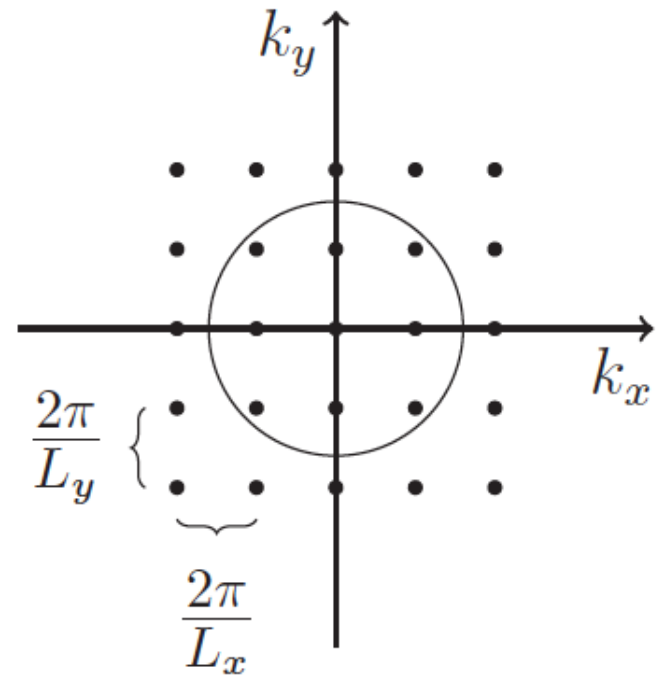
$$n = 1, 7, 19, 27, 33, 57, \ldots$$

- Taking spin and isospin quantum numbers into account we have the single-particle basis

$$|\mathbf{k}_n, s_z, t_z\rangle = |\mathbf{k}\rangle$$

- Closed shells for nuclear matter is then:

Example in 2D:



$$n = 4, 28, 76, 108, 132, 228, \ldots$$

Setting up the basis for nuclear matter with PBC

- Specify number nucleons in the reference state (only for closed shells: 4,28,76,... etc)
- Specify density $\rho = g_s k_F^3/(6\pi^2)$ or Fermi-momentum k_F
  (g_s = 2 for neutron matter and g_s = 4 for nuclear matter)
- Compute the volume of the cubic box according to

$$V = L^3 = A/\rho$$

- From L we can compute the lattice spacing:

$$\Delta k = 2\pi/L$$

- Specify n_{max} for the basis
- Generate a Fortran/python/C++ code that set up a single particle basis for PBC

Me: Run Fortran example in terminal window

Setting up the basis for nuclear matter with PBC

- Student task:
  - Code an algorithm for setting up a single-particle basis for neutron/nuclear matter for given density/Fermi momentum, number of nucleons, and n_{max}

A simple central nucleon-nucleon potential:

The Minnesota potential: central Gaussian potential and diagonal in spin and isospin.

$$V^c(r) = \frac{1}{2}\left(V_R + \frac{1}{2}(1+P_{12}^{\sigma})V_T + \frac{1}{2}(1-P_{12}^{\sigma})V_S\right)(1-P_{12}^{\sigma}P_{12}^{\tau})$$

The spin and isopsin exchange operators are given by:

$$P_{12}^{\sigma} = \frac{1}{2}(1+(\sigma_1\cdot\sigma_2)),\ P_{12}^{\tau} = \frac{1}{2}(1+(\tau_1\cdot\tau_2))$$

The potential in r-space:

$$V_R = V_{0R}\exp(-\kappa_R r_{12}^2)$$
$$V_T = -V_{0T}\exp(-\kappa_T r_{12}^2)$$
$$V_S = -V_{0S}\exp(-\kappa_S r_{12}^2)$$

The parameters of the potential are given by:

$$V_{0R} = 200\,\mathrm{MeV},\ \ \kappa_R = 1.487\,\mathrm{fm}^{-2}$$
$$V_{0T} = 178\,\mathrm{MeV},\ \ \kappa_T = 0.639\,\mathrm{fm}^{-2}$$
$$V_{0S} = 91.85\,\mathrm{MeV},\ \ \kappa_S = 0.465\,\mathrm{fm}^{-2}$$

Second quantized normal-ordered Hamiltonian:

$$H = E_0 + H_N \qquad H_N = \sum_{pq} \langle \mathbf{k}_p | f | \mathbf{k}_q \rangle : a_p^\dagger a_q :$$

$$+ \frac{1}{4} \sum_{pqrs} \langle \mathbf{k}_p \mathbf{k}_q | v | \mathbf{k}_r \mathbf{k}_s \rangle : a_p^\dagger a_q^\dagger a_s a_r :$$

The vacuum energy:

$$E_0 = \sum_i \langle \mathbf{k}_i | t | \mathbf{k}_i \rangle + \frac{1}{2} \sum_{i,j} \langle \mathbf{k}_i \mathbf{k}_j | V_{NN} | \mathbf{k}_i \mathbf{k}_j \rangle$$

The normal-ordered one-body part is given by:

$$\langle \mathbf{k}_p | f | \mathbf{k}_q \rangle = \langle \mathbf{k}_p | t | \mathbf{k}_q \rangle + \sum \langle \mathbf{k}_p \mathbf{k}_i | V_{\mathrm{NN}} | \mathbf{k}_q \mathbf{k}_i \rangle$$

The normal-ordered two-body part is given by:

$$\langle \mathbf{k}_p \mathbf{k}_q | v | \mathbf{k}_r \mathbf{k}_s \rangle = \langle \mathbf{k}_p \mathbf{k}_q | V_{\mathrm{NN}} | \mathbf{k}_r \mathbf{k}_s \rangle$$

Note: all two-body matrix elements are here assumed to be anti-symmetric

Outline Lecture 2

- Python script for setting up single particle states
- The Minnesota potential and computation of matrix elements in plane-wave basis
- Hartree-Fock for infinite matter using periodic boundary conditions
- Finite size effects and twist-averaging
- Going beyond mean-field
  - Many-body perturbation theory
  - Coupled-cluster in ladder approximation
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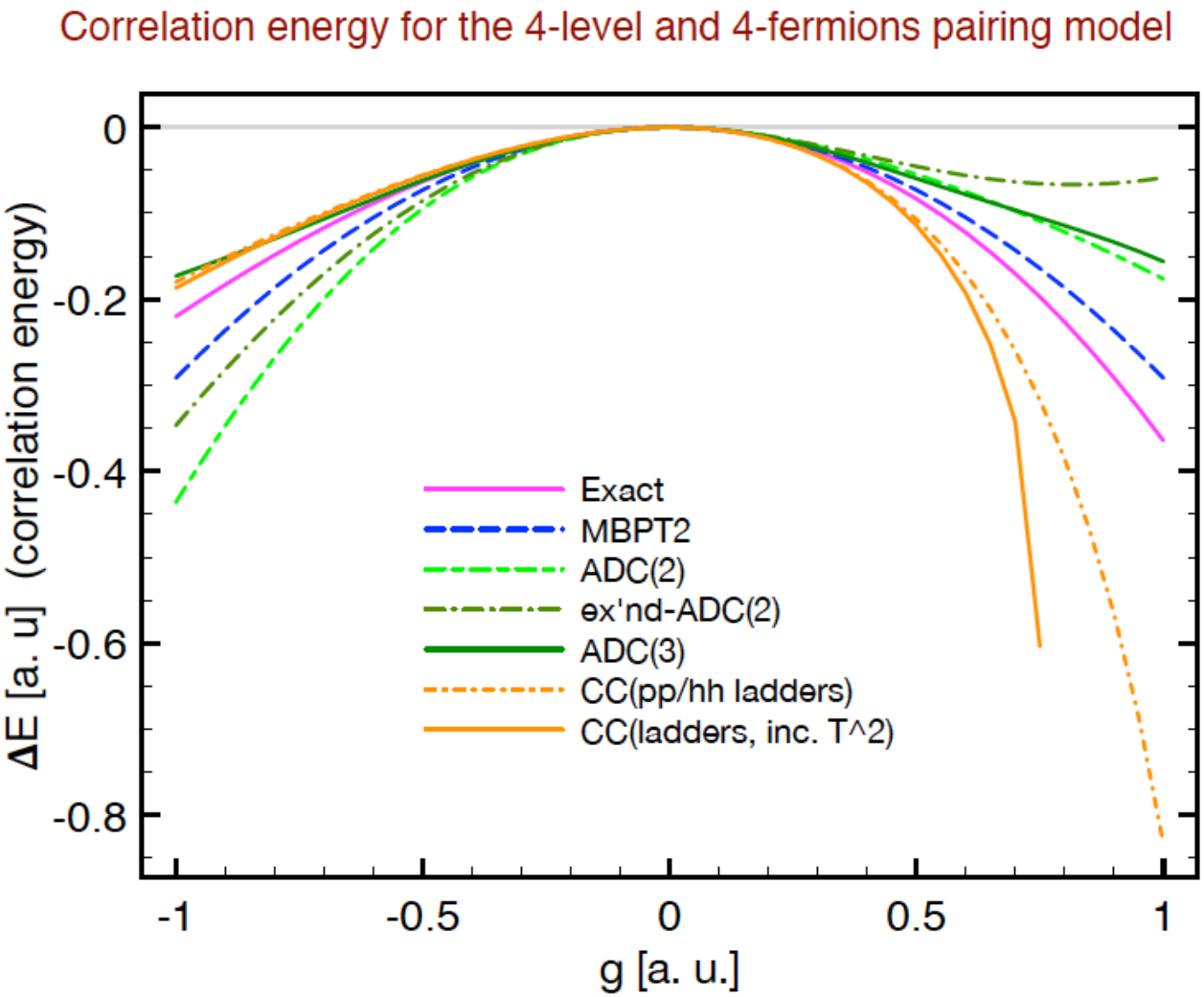
Benchmark results for the pairing model



G	ΔE_{CCD}
-1	-0.1764
-0.5	-0.0551
0	0.000
0.5	-0.1033
1.0	-0.5846

Can we understand the differences between ADC(2/3) and CCD?

What would be the leading order correction to CCD?

A simple central nucleon-nucleon potential:

The Minnesota potential: central Gaussian potential and diagonal in spin and isospin.

$$V^c(r) = \frac{1}{2}\left(V_R + \frac{1}{2}(1+P_{12}^{\sigma})V_T + \frac{1}{2}(1-P_{12}^{\sigma})V_S\right)(1-P_{12}^{\sigma}P_{12}^{\tau})$$

The spin and isopsin exchange operators are given by:

$$P_{12}^{\sigma} = \frac{1}{2}(1+(\sigma_1\cdot\sigma_2)),\ P_{12}^{\tau} = \frac{1}{2}(1+(\tau_1\cdot\tau_2))$$

The potential in r-space:

$$V_R = V_{0R}\exp(-\kappa_R r_{12}^2)$$
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Second quantized normal-ordered Hamiltonian:

Matrix elements of kinetic energy: $$\langle \mathbf{k}_p | t | \mathbf{k}_q \rangle = \frac{\hbar^2}{2m} \vec{k}_p^2 \delta_{pq}$$

Matrix elements of a Gaussian nucleon-nucleon interaction are: $$V_R = V_0 \exp(-\alpha r_{12}^2)$$

$$\langle \mathbf{k}_p \mathbf{k}_q | v | \mathbf{k}_r \mathbf{k}_s \rangle = \frac{V_0}{L^3} \left(\frac{\pi}{\alpha} \right)^{3/2} \exp(-q^2/4\alpha) \delta_{\vec{k}_p + \vec{k}_q, \vec{k}_r + \vec{k}_s}$$

q is the relative momentum transfer: $$\mathbf{q} = \mathbf{p} - \mathbf{p}'$$

Relative momenta are defined: $$\mathbf{p} = \frac{1}{2}(\mathbf{k}_p - \mathbf{k}_q)$$ $$\mathbf{p}' = \frac{1}{2}(\mathbf{k}_r - \mathbf{k}_s)$$

Anti-symmetric matrix elements are then computed:

$$\langle \mathbf{k}_p \mathbf{k}_q | v | \mathbf{k}_r \mathbf{k}_s \rangle_{AS} = \langle \mathbf{k}_p \mathbf{k}_q | v | \mathbf{k}_r \mathbf{k}_s \rangle - \langle \mathbf{k}_p \mathbf{k}_q | v | \mathbf{k}_s \mathbf{k}_r \rangle$$

Note periodic boundary conditions ensures that momentum is conserved: $$\mathbf{k}_p + \mathbf{k}_q = \mathbf{k}_r + \mathbf{k}_s$$

Matrix elements of the Minnesota potential

$$\langle \mathbf{k}_p \mathbf{k}_q | v | \mathbf{k}_r \mathbf{k}_s \rangle =$$
$$\langle \mathbf{k}_p \mathbf{k}_q | \frac{1}{2} \left(V_R + \frac{1}{2} V_T + \frac{1}{2} V_S \right) | \mathbf{k}_r \mathbf{k}_s \rangle +$$
$$\langle \mathbf{k}_p \mathbf{k}_q | \frac{1}{4} \left(V_T - V_S \right) P_{12}^{\sigma} | \mathbf{k}_r \mathbf{k}_s \rangle -$$
$$\langle \mathbf{k}_p \mathbf{k}_q | \frac{1}{2} \left(V_R + \frac{1}{2} V_T + \frac{1}{2} V_S \right) P_{12}^{\sigma} P_{12}^{\tau} | \mathbf{k}_r \mathbf{k}_s \rangle -$$
$$\langle \mathbf{k}_p \mathbf{k}_q | \frac{1}{4} \left(V_T - V_S \right) P_{12}^{\tau} | \mathbf{k}_r \mathbf{k}_s \rangle$$

Matrix elements of the spin exchange operator are (and similarly for the isospin):

$$\langle \sigma_p \sigma_q | P_{12}^{\sigma} | \sigma_r \sigma_s \rangle = \delta_{\sigma_p, \sigma_s} \delta_{\sigma_q, \sigma_r} \qquad P_{12}^2 = 1$$

Setting up the basis for nuclear matter with PBC

- Student task:
  - Derive a programmable expression for the Minnesota potential in a plane-wave basis for periodic boundary conditions:

$$\langle \mathbf{k}_p \mathbf{k}_q | v | \mathbf{k}_r \mathbf{k}_s \rangle$$

Hartree-Fock for infinite matter

Hartree-Fock computed using PBC:

$$E_0 = \sum_i \langle \mathbf{k}_i | t | \mathbf{k}_i \rangle + \frac{1}{2} \sum_{i,j} \langle \mathbf{k}_i \mathbf{k}_j | V_{NN} | \mathbf{k}_i \mathbf{k}_j \rangle$$

Hartree-Fock computed in relative center-of-mass coordinates for a central potential:

$$\frac{E_0}{A} = \frac{3\hbar^2 k_F^2}{10m} + \frac{1}{(2\pi)^6} \frac{V}{2\rho} \sum_{t_{z_1} t_{z_2}} \sum_{s_{z_1} s_{z_2}} \int_0^{k_F} d\vec{k}_1 \int_0^{k_F} d\vec{k}_2 \, \langle \mathbf{k_1 k_2} | v | \mathbf{k_1 k_2} \rangle$$

Remember: $|\mathbf{k}_i\rangle = |\vec{k}_i, s_z, t_z\rangle$ and: $A = \rho V$

And matrix elements are anti-symmetric:

$$\langle \mathbf{k_1 k_2} | v | \mathbf{k_1 k_2} \rangle = \langle \mathbf{k_1 k_2} | v | \mathbf{k_1 k_2} \rangle - \langle \mathbf{k_1 k_2} | v | \mathbf{k_2 k_1} \rangle$$

Hartree-Fock for infinite matter

Computing the six dimensional potential energy term for HF:
can be computed "brute" force (but there is a simpler way).

$$\frac{1}{(2\pi)^6}\frac{V}{2\rho}\sum_{t_{z_1}t_{z_2}}\sum_{s_{z_1}s_{z_2}}\int_0^{k_F} d\vec{k}_1\int_0^{k_F} d\vec{k}_2\,\langle \mathbf{k_1}\mathbf{k_2}|v|\mathbf{k_1}\mathbf{k_2}\rangle$$

Note the interaction only depends on the momentum transfer squared q^2

$$q^2 = p^2 - p'^2 - 2pp'cos(\theta)$$

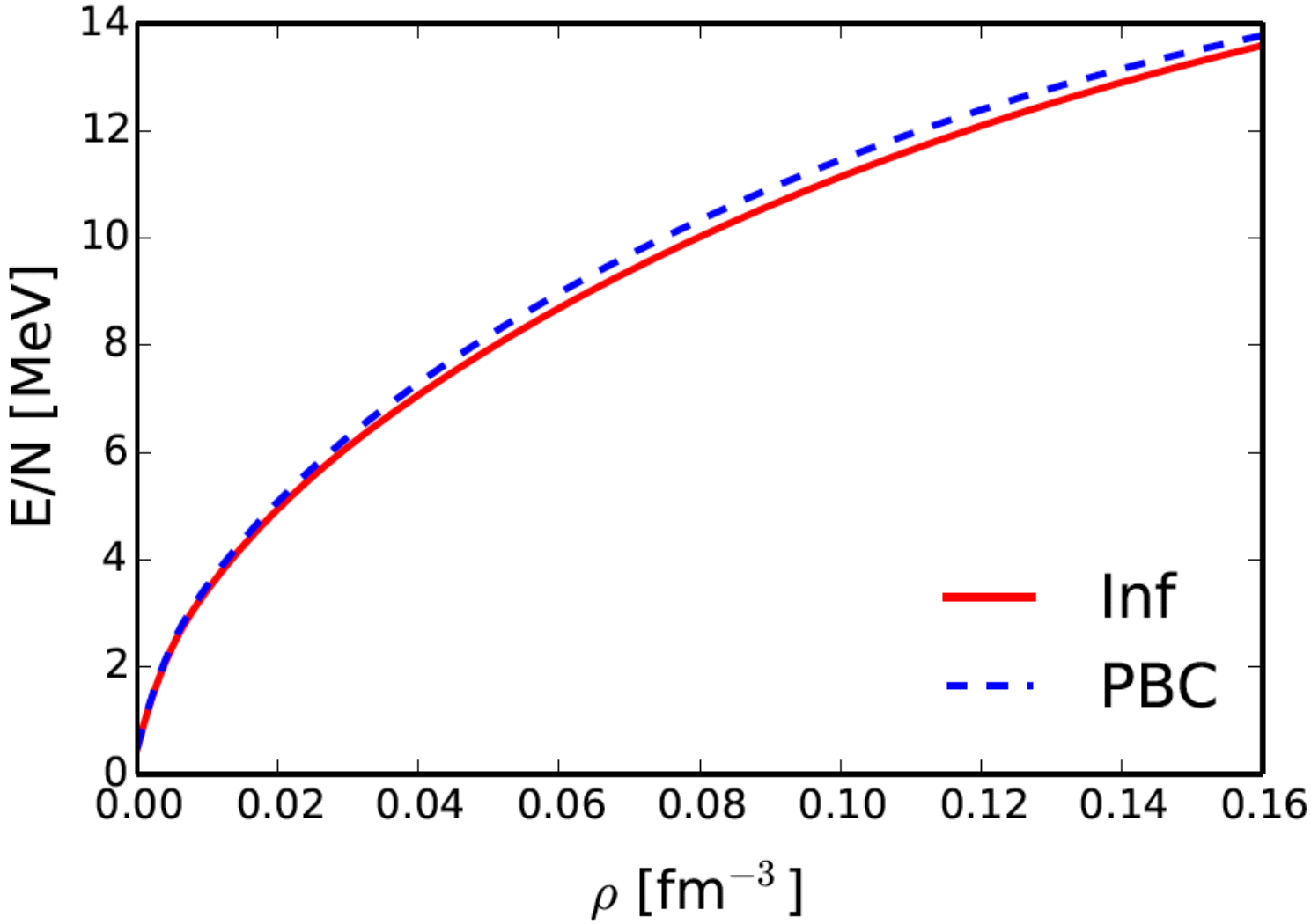
$$\mathbf{p} = \frac{1}{2}(\mathbf{k}_p - \mathbf{k}_q)$$

$$\mathbf{p}' = \frac{1}{2}(\mathbf{k}_r - \mathbf{k}_s)$$

Hint: We can write the six dimensional integral as a three-dimensional integral by fixing one momenta along the z-axis and integrating over 3 angles (see notes on infinite matter at the github address of the course)

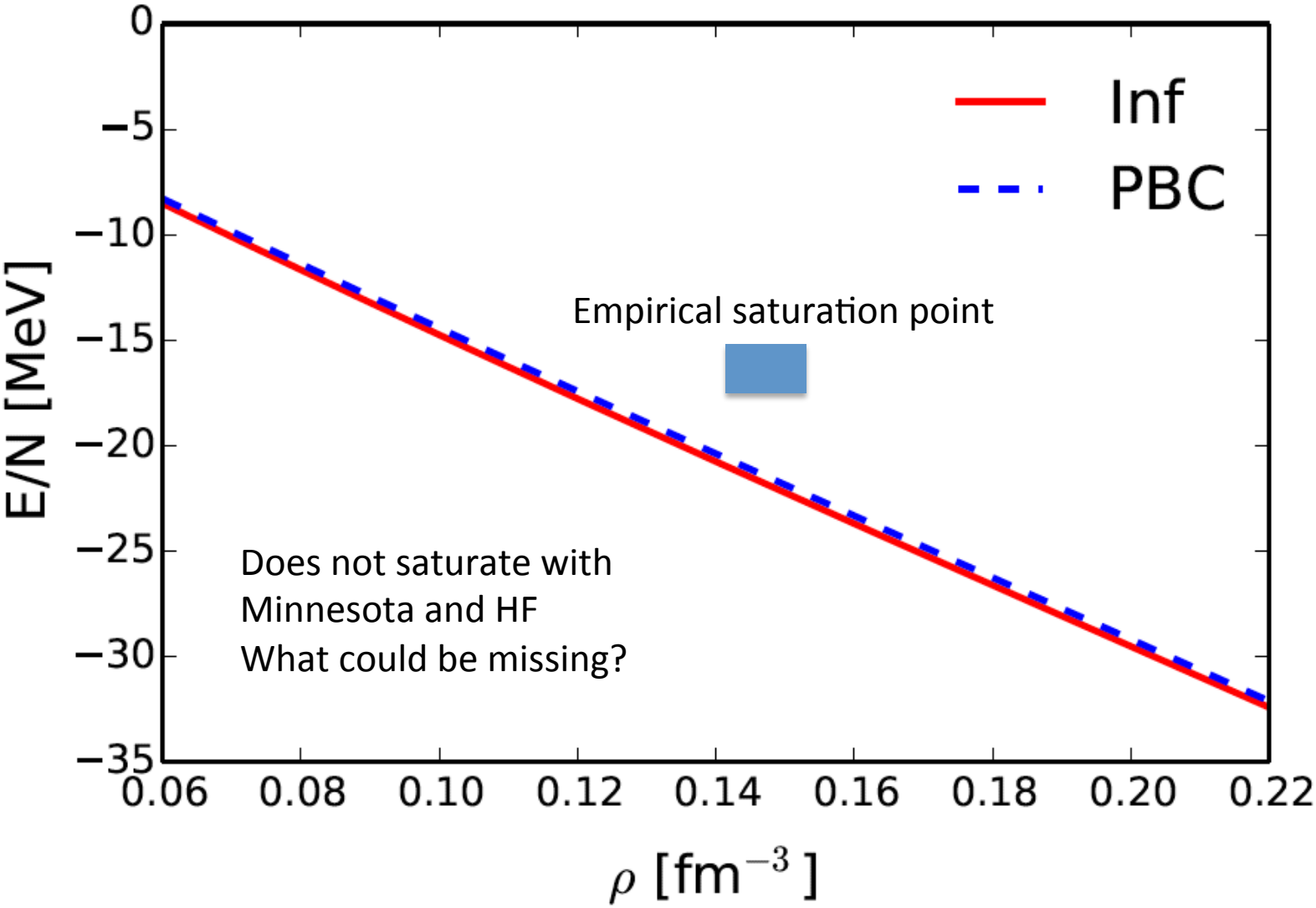
Hartree-Fock for infinite matter

Benchmark for Hartree-Fock energy in pure neutron matter for the Minnesota potential. PBC used 14 particles and $n_{max} = 3$.



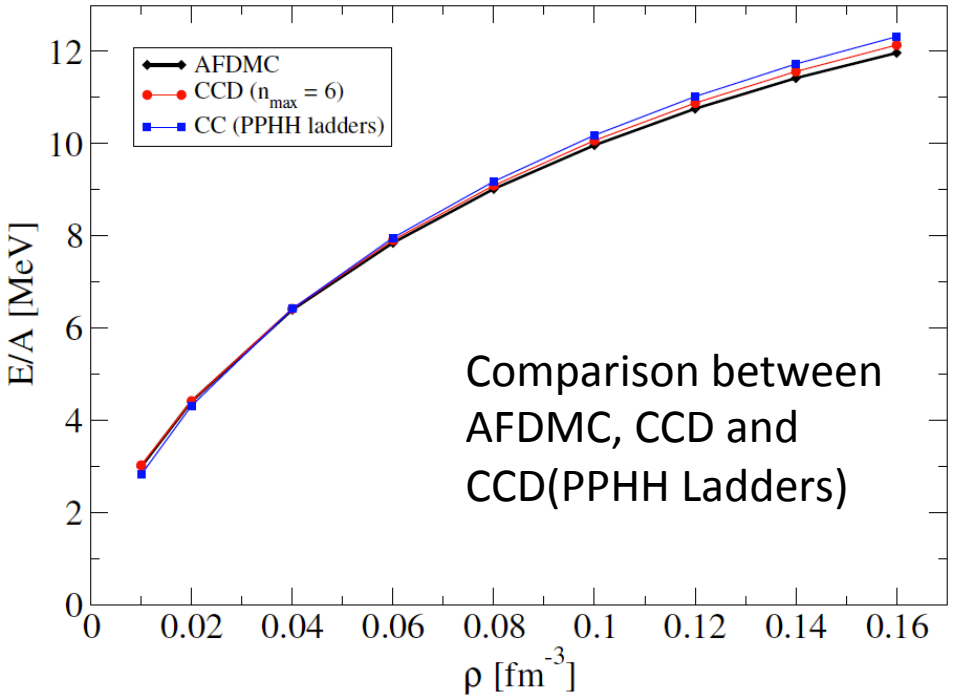
Hartree-Fock for infinite matter

Benchmark for Hartree-Fock energy in symmetric neutron matter for the Minnesota potential. PBC used 28 particles and $n_{max} = 3$.



Benchmark results for the Minnesota potential

Benchmark results (Table below) for Hartree-Fock, MBPT2 and CCD energy in pure neutron matter (PNM) and symmetric nuclear matter (SNM) with the Minnesota potential. Here we used PBC with 14 particles for PNM and 28 particles for SNM with a model space size given by n_{max} = 2 (this gives 250 states for PNM and 500 states for SNM).

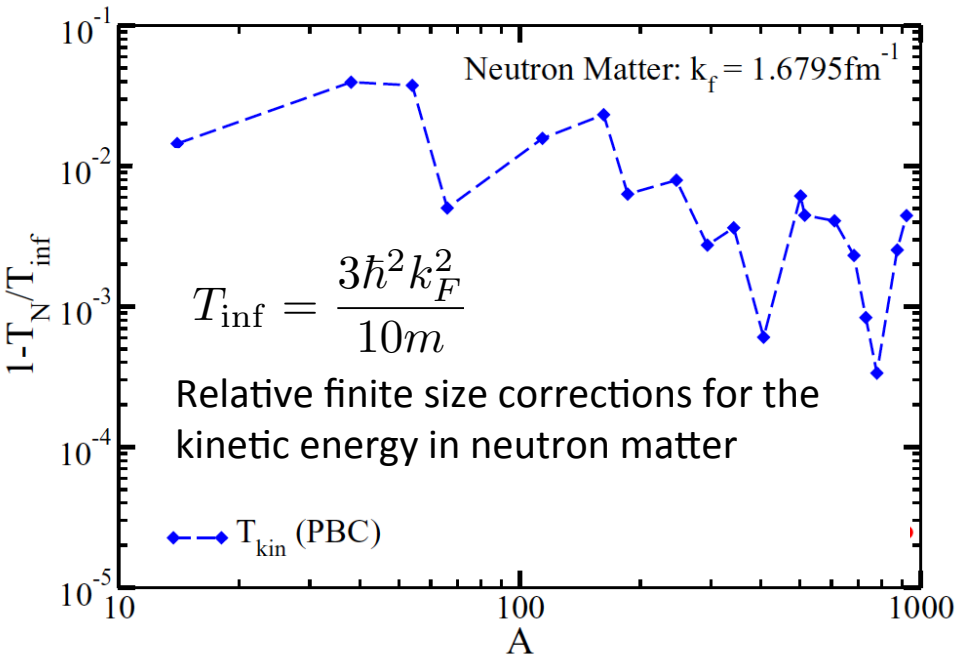


Type	k_F	ρ	*E0/A*	*MBPT2/A*	*CCD/A*
PNM	1.33302	0.08	10.33372	9.70395	9.69991
PNM	1.43595	0.10	11.45846	10.74053	10.74307
PNM	1.52593	0.12	12.38970	11.59136	11.59903
SNM	1.33302	0.16	-23.33771	-26.34531	-28.26330
SNM	1.38640	0.18	-26.26943	-29.27810	-30.63909
SNM	1.43595	0.20	-29.19769	-32.20519	-33.22750

Setting up the basis for nuclear matter with PBC

- Student task:
  - Code a program for computing the Hartree-Fock energy per nucleon in infinite neutron/nuclear matter for given density/Fermi momentum using the Minnesota nucleon-nucleon potential
  - Study how E/A changes with density/Fermi momentum
  - Study finite size effects by varying the particle number
  - Benchmark against Hartree-Fock computed in relative center-of-mass coordinates

Twist averaged periodic boundary conditions



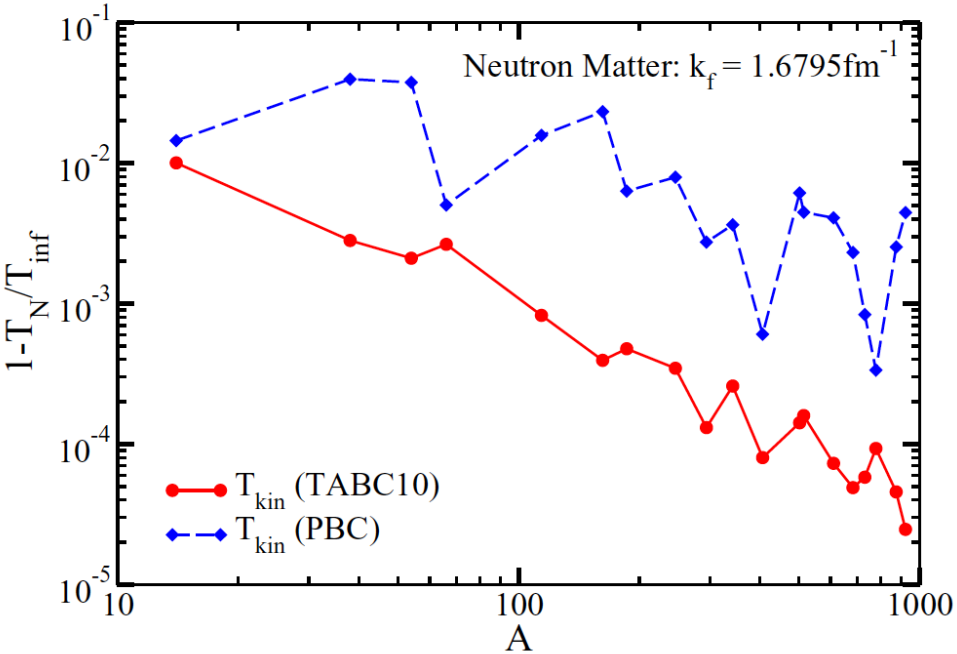
- How to quantify error from shell oscillations/finite size effects?
- By increasing number of nucleons we don't see a systematic and smooth convergence to the thermodynamic limit
- Comparing the kinetic energy computed with PBC and in the thermodynamic limit we can find an optimal number of particles
- Is there a more systematic way?
  Yes: Use twist-averaged PBC.

"Twist averaged" boundary conditions: average over all possible phases of Bloch waves. Exactly removes finite size effects for the free Fermi gas:

$$k_{n_i} = \frac{(2\pi n_i + \theta_i)}{L} \qquad \psi_k(x+L) = e^{i\theta}\psi_k(x)$$

[Gros, Z. Phys. B 86, 359 (1992); Lin, Zong, and Ceperley, Phys. Rev. E 64, 016702 (2001)]
Discrete momenta are

Twist averaged periodic boundary conditions



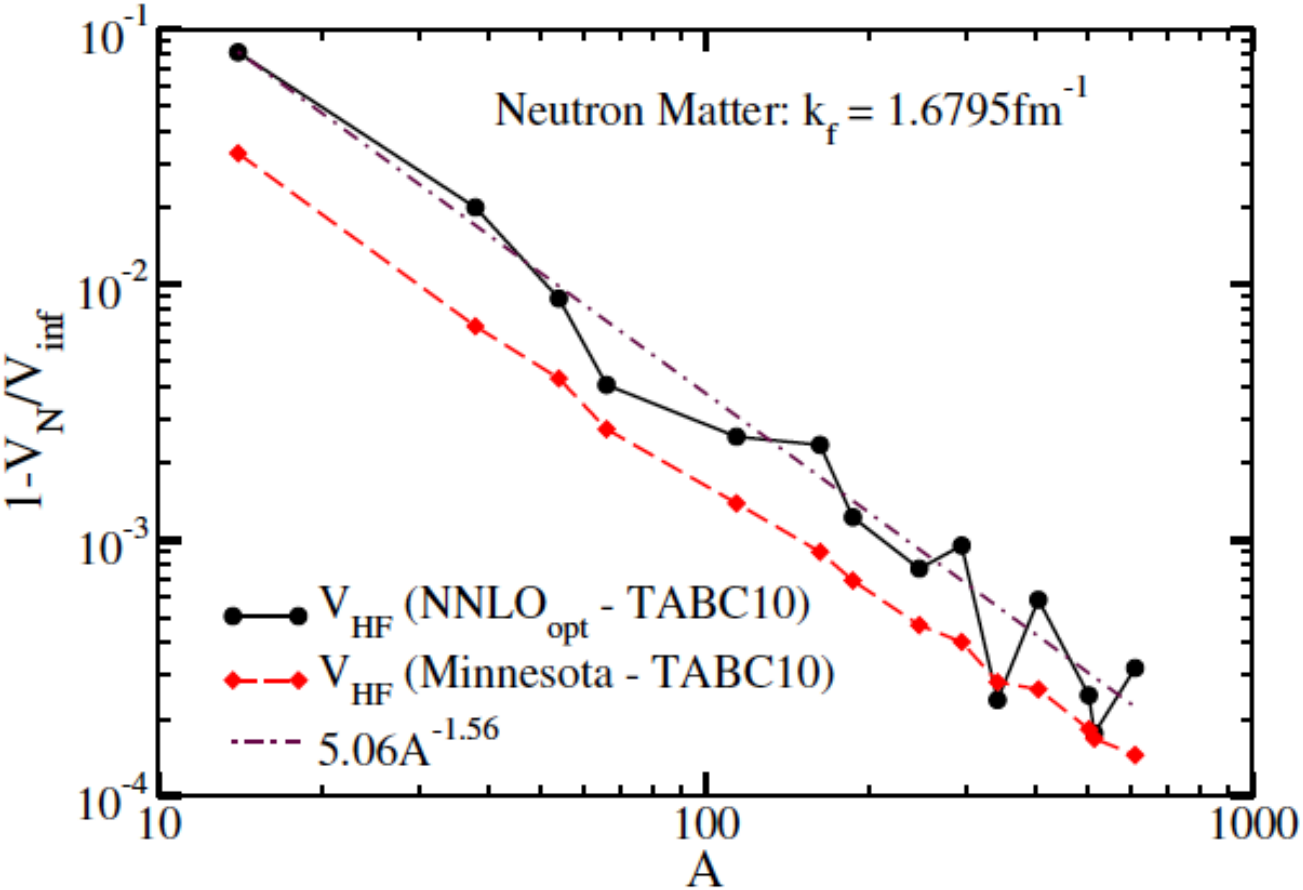
- Finite size effects for kinetic energy in neutron matter for PBC and TAPBC
- With TAPBC we obtain a smooth/systematic convergence to thermodynamic limit

- Choose a mesh (e.g. Gauss-Legendre) for the twist angles $\theta_{x,y,z}$ in the interval: $[0, \pi]$
- Loop over mesh in x,y,z and compute kinetic and hartree-fock energy
- Very costly: for 10 points you need to compute the energy at one density 10^3 times.
- The final energy computed with TAPBC is

$$E_0^{TA} = E_0^{TA} + \left(\frac{1}{\pi^3}\right) w_{\theta_x} w_{\theta_y} w_{\theta_z} E_0(\theta_x, \theta_y, \theta_z)$$

Twist averaged peridodic boundary conditions

Relative finite size corrections for the Hartree-Fock energy of pure neutron matter with the Minnesota potential



N	n_θ	Method	E_0
14	2	TA	11.031
14	6	TA	11.046
14	10	TA	11.049
14	14	TA	11.033
14	1	PBC	11.458
66	1	PBC	10.980
66	10	TA	11.175
		Inf	**11.141**

$$\rho = 0.10\ \mathrm{fm}^{-3}, \quad n_{\max} = 3$$

Quantifying errors from finite size effects

- Student task:
  - Implement twist-averaged periodic boundary conditions in pure neutron matter for the kinetic energy (possibly HF)
  - Study convergence to thermodynamic limit with number of closed shell neutrons and number meshpoints for the twist angles

Going beyond mean-field: MBPT2

- Correlations beyond mean-field are important in nuclear physics (strongly correlated many-body problem)
- First attempt is many-body perturbation theory at second order

$$E_{\mathrm{MBPT2}} = E_0 + \frac{1}{4}\sum_{ijab}\langle \mathbf{k}_i\mathbf{k}_j|v|\mathbf{k}_a\mathbf{k}_b\rangle\langle \mathbf{k}_a\mathbf{k}_b|t^0|\mathbf{k}_i\mathbf{k}_j\rangle$$

Here a,b,c, are orbitals above the Fermi level (unoccopied) and i,j,k… are orbitals below the Fermi level (occupied)

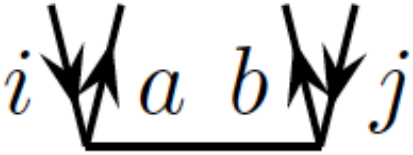
Hartree-Fock energy (1st order MBPT):

$$E_0 = \sum_i \langle \mathbf{k}_i|t|\mathbf{k}_i\rangle + \frac{1}{2}\sum_{i,j}\langle \mathbf{k}_i\mathbf{k}_j|V_{NN}|\mathbf{k}_i\mathbf{k}_j\rangle$$

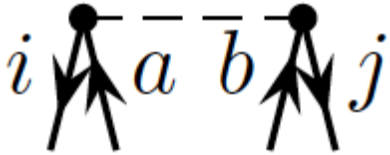
The t^0 amplitudes are:

$$\langle \mathbf{k}_a\mathbf{k}_b|t^0|\mathbf{k}_i\mathbf{k}_j\rangle = \frac{\langle \mathbf{k}_a\mathbf{k}_b|v|\mathbf{k}_i\mathbf{k}_j\rangle}{f_{ii}+f_{jj}-f_{aa}-f_{bb}} \qquad f_{pq} = \langle \mathbf{k}_p|f|\mathbf{k}_q\rangle$$

Brief introduction to coupled-cluster diagrams



$= \langle ab|t|ij\rangle$

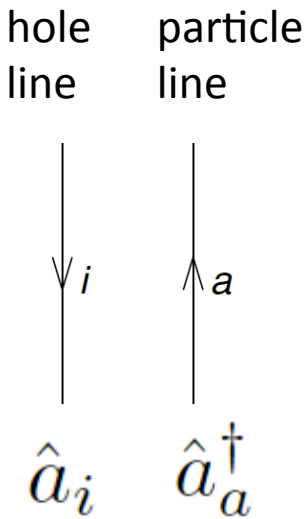


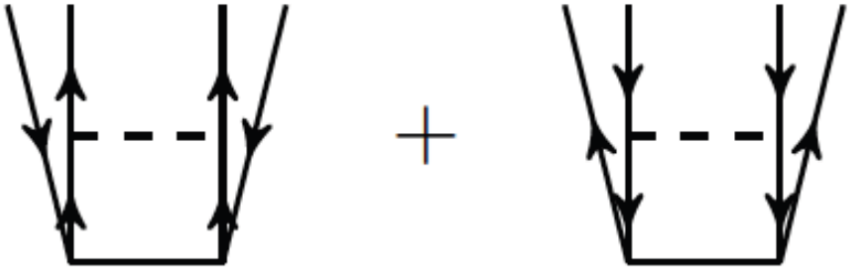
$= \langle ij|v|ab\rangle$

- Assign labels to particle and hole lines
- Matrix elements are in the order

$$\langle \mathrm{left}_{\mathrm{out}}, \mathrm{right}_{\mathrm{out}}|v|\mathrm{left}_{\mathrm{in}}, \mathrm{right}_{\mathrm{in}}\rangle$$

- Each diagram gets a factor ½ for equivalent lines
- Each diagram gets the phase $(-1)^{h+l}$
- Each diagram is anti-symmetrized in out/in-going lines

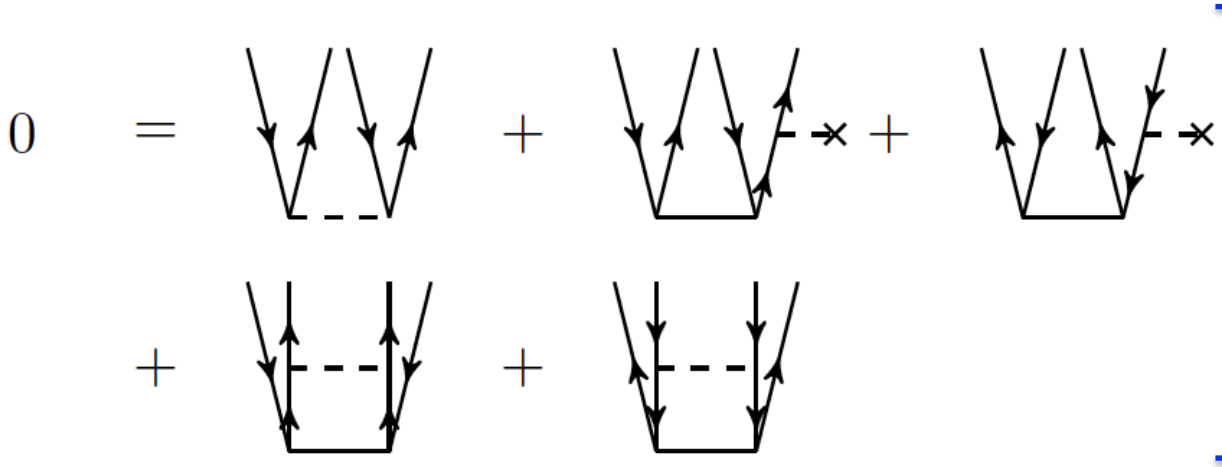




$$= \frac{1}{2}\sum_{cd} \langle \mathbf{k}_a\mathbf{k}_b|v|\mathbf{k}_c\mathbf{k}_d\rangle \langle \mathbf{k}_c\mathbf{k}_d|t|\mathbf{k}_i\mathbf{k}_j\rangle$$

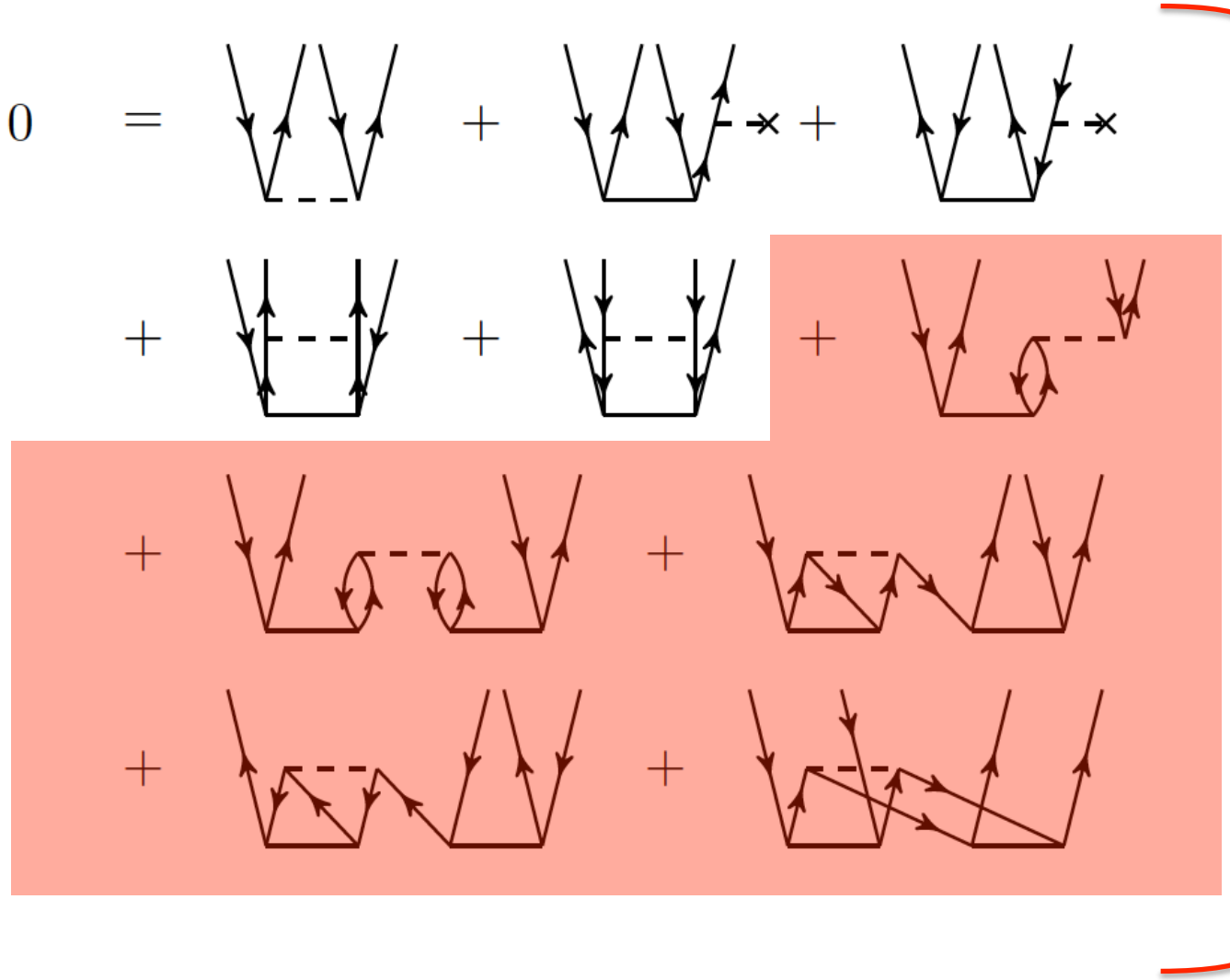
$$+ \frac{1}{2}\sum_{kl} \langle \mathbf{k}_a\mathbf{k}_b|t|\mathbf{k}_k\mathbf{k}_l\rangle \langle \mathbf{k}_k\mathbf{k}_l|v|\mathbf{k}_i\mathbf{k}_j\rangle$$

Going beyond mean-field with coupled-cluster method



CCD(pphh)
Brueckner HF

Going beyond mean-field with coupled-cluster method



CCD

Going beyond mean-field: CCD_{ladd}

Note: For infinite nucleonic matter there are no singles excitations due to momentum conservation

The CCD equations are given by:

$$
\begin{aligned}
0 = & \langle \mathbf{k}_a \mathbf{k}_b | v | \mathbf{k}_i \mathbf{k}_j \rangle \\
& + P(ab) \sum_c \langle \mathbf{k}_b | f | \mathbf{k}_c \rangle \langle \mathbf{k}_a \mathbf{k}_c | t | \mathbf{k}_i \mathbf{k}_j \rangle \\
& - P(ij) \sum_k \langle \mathbf{k}_k | f | \mathbf{k}_j \rangle \langle \mathbf{k}_a \mathbf{k}_b | t | \mathbf{k}_i \mathbf{k}_k \rangle \\
& + \frac{1}{2} \sum_{cd} \langle \mathbf{k}_a \mathbf{k}_b | v | \mathbf{k}_c \mathbf{k}_d \rangle \langle \mathbf{k}_c \mathbf{k}_d | t | \mathbf{k}_i \mathbf{k}_j \rangle \\
& + \frac{1}{2} \sum_{kl} \langle \mathbf{k}_a \mathbf{k}_b | t | \mathbf{k}_k \mathbf{k}_l \rangle \langle \mathbf{k}_k \mathbf{k}_l | v | \mathbf{k}_i \mathbf{k}_j \rangle
\end{aligned}
$$

The most costly term to evaluate in the CCD approximation. Computational cost is (naively):

$$n_u^4 n_o^2$$

But: Due to momentum conservation the cost is reduced to

$$n_u^3 n_o$$

Going beyond mean-field: CCD_{ladd}

$$D_{ij}^{ab} = f_{ii} + f_{jj} - f_{aa} - f_{bb}$$

$$\begin{aligned} D_{ij}^{ab} \langle \mathbf{k}_a \mathbf{k}_b | t | \mathbf{k}_i \mathbf{k}_j \rangle &= \langle \mathbf{k}_a \mathbf{k}_b | v | \mathbf{k}_i \mathbf{k}_j \rangle \\ &+ P(ab) \sum_{c \neq a} \langle \mathbf{k}_b | f | \mathbf{k}_c \rangle \langle \mathbf{k}_a \mathbf{k}_c | t | \mathbf{k}_i \mathbf{k}_j \rangle \\ &- P(ij) \sum_{k \neq i} \langle \mathbf{k}_k | f | \mathbf{k}_j \rangle \langle \mathbf{k}_a \mathbf{k}_b | t | \mathbf{k}_i \mathbf{k}_k \rangle \\ &+ \frac{1}{2} \sum_{cd} \langle \mathbf{k}_a \mathbf{k}_b | v | \mathbf{k}_c \mathbf{k}_d \rangle \langle \mathbf{k}_c \mathbf{k}_d | t | \mathbf{k}_i \mathbf{k}_j \rangle \\ &+ \frac{1}{2} \sum_{kl} \langle \mathbf{k}_a \mathbf{k}_b | t | \mathbf{k}_k \mathbf{k}_l \rangle \langle \mathbf{k}_k \mathbf{k}_l | v | \mathbf{k}_i \mathbf{k}_j \rangle \end{aligned}$$

Solve non-linear CCD equations iteratively starting from the MBPT2 ansatz for t^0
Convergence is improve by using a linear mixing between new and old amplitudes:

$$t^{(i)} = \alpha t^{(i)} + (1 - \alpha) t^{(i-1)}$$

Once the t-amplitudes are converged compute the CCD energy:

$$E_{\mathrm{CCD}} = E_0 + \frac{1}{4} \sum_{ijab} \langle \mathbf{k}_i \mathbf{k}_j | v | \mathbf{k}_a \mathbf{k}_b \rangle \langle \mathbf{k}_a \mathbf{k}_b | t | \mathbf{k}_i \mathbf{k}_j \rangle$$

Solving the CCD_{ladd} equations efficiently

$$\frac{1}{2}\sum_{cd}\langle \underbrace{\mathbf{k}_a\mathbf{k}_b}_{A}|v|\underbrace{\mathbf{k}_c\mathbf{k}_d}_{C}\rangle\,\langle \underbrace{\mathbf{k}_c\mathbf{k}_d}_{C}|t|\underbrace{\mathbf{k}_i\mathbf{k}_j}_{I}\rangle$$

We can write the tensor contractions as a matrix-matrix multiplication:

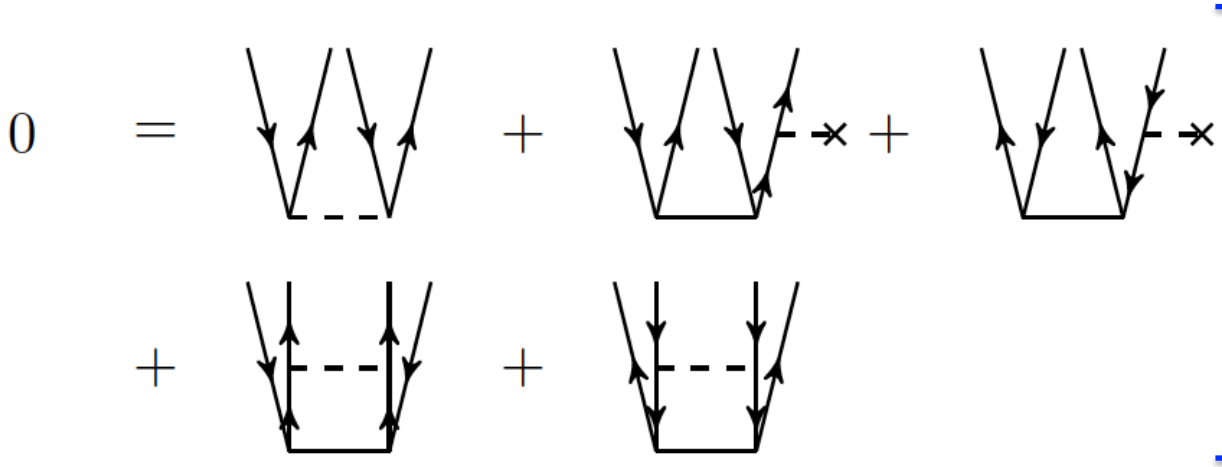
$$\frac{1}{2}\sum_{C}\langle A|v|C\rangle\langle C|t|I\rangle$$

Matrix-matrix multiplications can be efficiently solved by using linear algebra libraries such as LAPACK (Linear Algebra PACKage) and BLAS (Basic Linear Algebra Subprograms) routines.

Going beyond the mean-field

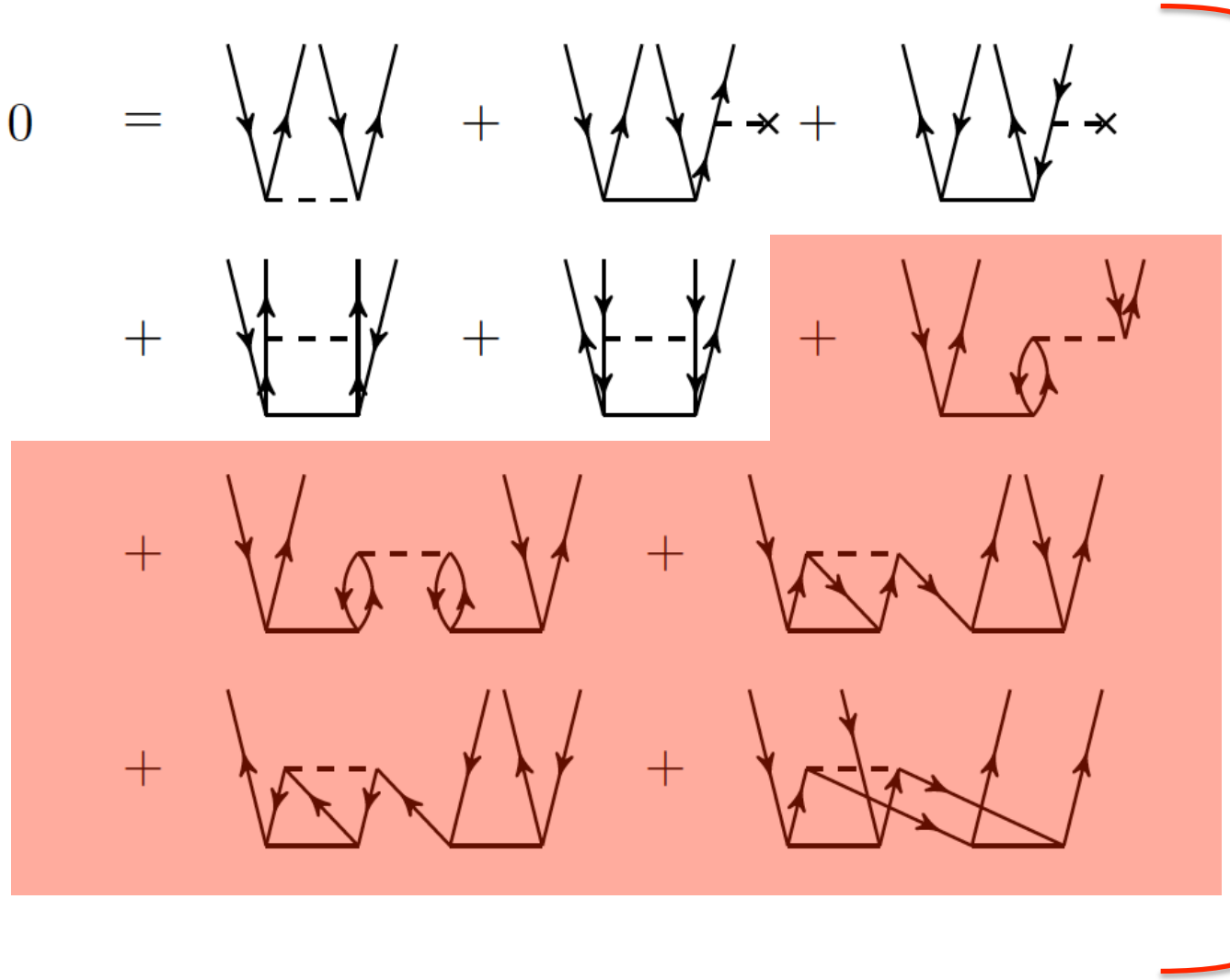
- Student task:
  - Implement MBPT2 for pure neutron matter and symmetric nuclear matter using PBC and the Minnesota potential
  - Code coupled-cluster for neutron matter and symmetric nuclear matter keeping only particle-particle and hole-hole ladder terms (CCD_{ladd}) and the Minnesota potential

Going beyond mean-field with coupled-cluster method



CCD(pphh)
Brueckner HF

Going beyond mean-field with coupled-cluster method



CCD

Going beyond mean-field: CCD

The full CCD equations in factorized form:

$$
\begin{aligned}
0 = & \langle \mathbf{k}_a \mathbf{k}_b | v | \mathbf{k}_i \mathbf{k}_j \rangle \\
& + P(ab) \sum_c \langle \mathbf{k}_b | \chi | \mathbf{k}_c \rangle \langle \mathbf{k}_a \mathbf{k}_c | t | \mathbf{k}_i \mathbf{k}_j \rangle \\
& - P(ij) \sum_k \langle \mathbf{k}_k | \chi | \mathbf{k}_j \rangle \langle \mathbf{k}_a \mathbf{k}_b | t | \mathbf{k}_i \mathbf{k}_k \rangle \\
& + \frac{1}{2} \sum_{cd} \langle \mathbf{k}_a \mathbf{k}_b | \chi | \mathbf{k}_c \mathbf{k}_d \rangle \langle \mathbf{k}_c \mathbf{k}_d | t | \mathbf{k}_i \mathbf{k}_j \rangle \\
& + \frac{1}{2} \sum_{kl} \langle \mathbf{k}_a \mathbf{k}_b | t | \mathbf{k}_k \mathbf{k}_l \rangle \langle \mathbf{k}_k \mathbf{k}_l | \chi | \mathbf{k}_i \mathbf{k}_j \rangle \\
& + P(ij) P(ab) \sum_{kc} \langle \mathbf{k}_a \mathbf{k}_c | t | \mathbf{k}_i \mathbf{k}_k \rangle \langle \mathbf{k}_k \mathbf{k}_b | \chi | \mathbf{k}_c \mathbf{k}_j \rangle
\end{aligned}
$$

Going beyond mean-field: CCD

One-body intermediates:

$$\langle \mathbf{k}_b|\chi|\mathbf{k}_c\rangle = \langle \mathbf{k}_b|f|\mathbf{k}_c\rangle - \frac{1}{2}\sum_{kld} \langle \mathbf{k}_b\mathbf{k}_d|t|\mathbf{k}_k\mathbf{k}_l\rangle \langle \mathbf{k}_k\mathbf{k}_l|v|\mathbf{k}_c\mathbf{k}_d\rangle$$

$$\langle \mathbf{k}_k|\chi|\mathbf{k}_j\rangle = \langle \mathbf{k}_k|f|\mathbf{k}_j\rangle + \frac{1}{2}\sum_{kcd} \langle \mathbf{k}_k\mathbf{k}_l|v|\mathbf{k}_c\mathbf{k}_d\rangle \langle \mathbf{k}_c\mathbf{k}_d|t|\mathbf{k}_j\mathbf{k}_l\rangle$$

Two-body intermediates:

$$\langle \mathbf{k}_k\mathbf{k}_l|\chi|\mathbf{k}_i\mathbf{k}_j\rangle = \langle \mathbf{k}_k\mathbf{k}_l|v|\mathbf{k}_i\mathbf{k}_j\rangle + \frac{1}{2}\sum_{cd} \langle \mathbf{k}_k\mathbf{k}_l|v|\mathbf{k}_c\mathbf{k}_d\rangle \langle \mathbf{k}_c\mathbf{k}_d|t|\mathbf{k}_i\mathbf{k}_j\rangle$$

$$\langle \mathbf{k}_k\mathbf{k}_b|\chi|\mathbf{k}_c\mathbf{k}_j\rangle = \langle \mathbf{k}_k\mathbf{k}_b|v|\mathbf{k}_c\mathbf{k}_j\rangle + \sum_{ld} \langle \mathbf{k}_k\mathbf{k}_l|v|\mathbf{k}_c\mathbf{k}_d\rangle \langle \mathbf{k}_c\mathbf{k}_d|t|\mathbf{k}_l\mathbf{k}_j\rangle$$

$$\langle \mathbf{k}_a\mathbf{k}_b|\chi|\mathbf{k}_c\mathbf{k}_d\rangle = \langle \mathbf{k}_a\mathbf{k}_b|v|\mathbf{k}_c\mathbf{k}_d\rangle$$

Why use intermediates?

$$n_u^3 n_o^3 + n_u^2 n_o^2 + n_u^3 n_o^4 \qquad n_u \gg n_o$$

$$\sum_{kc} \langle \mathbf{k}_a \mathbf{k}_c | t | \mathbf{k}_i \mathbf{k}_k \rangle \langle \mathbf{k}_k \mathbf{k}_b | \chi | \mathbf{k}_c \mathbf{k}_j \rangle$$

$$= \sum_{kc} \langle \mathbf{k}_a \mathbf{k}_c | t | \mathbf{k}_i \mathbf{k}_k \rangle \langle \mathbf{k}_k \mathbf{k}_b | v | \mathbf{k}_c \mathbf{k}_j \rangle$$

$$+ \frac{1}{2} \sum_{kcld} \langle \mathbf{k}_a \mathbf{k}_c | t | \mathbf{k}_i \mathbf{k}_k \rangle \langle \mathbf{k}_k \mathbf{k}_l | v | \mathbf{k}_c \mathbf{k}_d \rangle \langle \mathbf{k}_b \mathbf{k}_d | t | \mathbf{l}_i \mathbf{k}_j \rangle$$

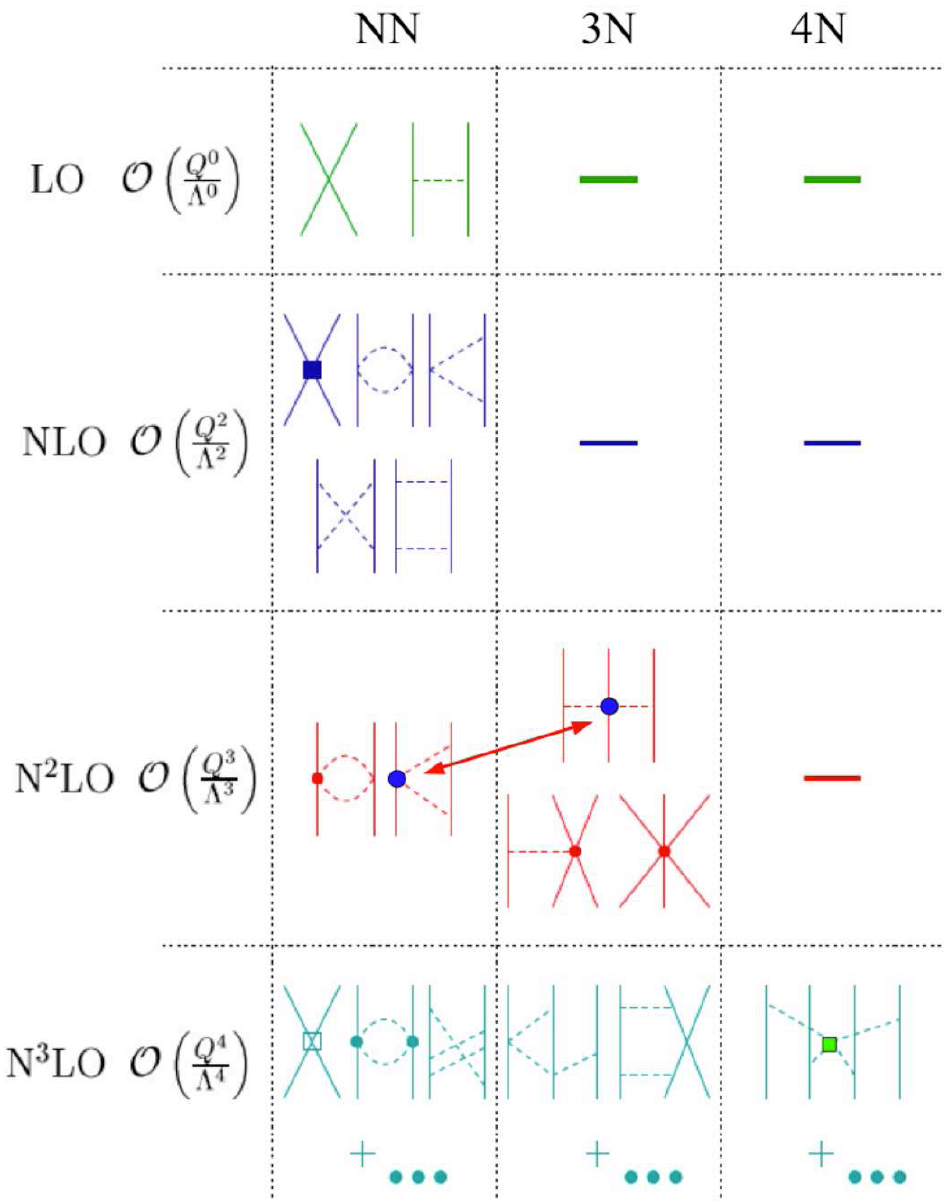
$$n_u^3 n_o^3 + n_u^4 n_o^4$$

Going beyond the mean-field

- Student task:
  - Derive the CCD equations from the CCD diagrams using the diagrams rules
  - Write the CCD equations in a factorized form using intermediates
  - Implement CCD for symmetric nuclear matter and pure neutron matter
  - Do a comparison between HF, MBPT2, CCD_{ladd} and CCD in pure neutron matter and nuclear matter around saturation density

Nuclear forces from chiral effective field theory

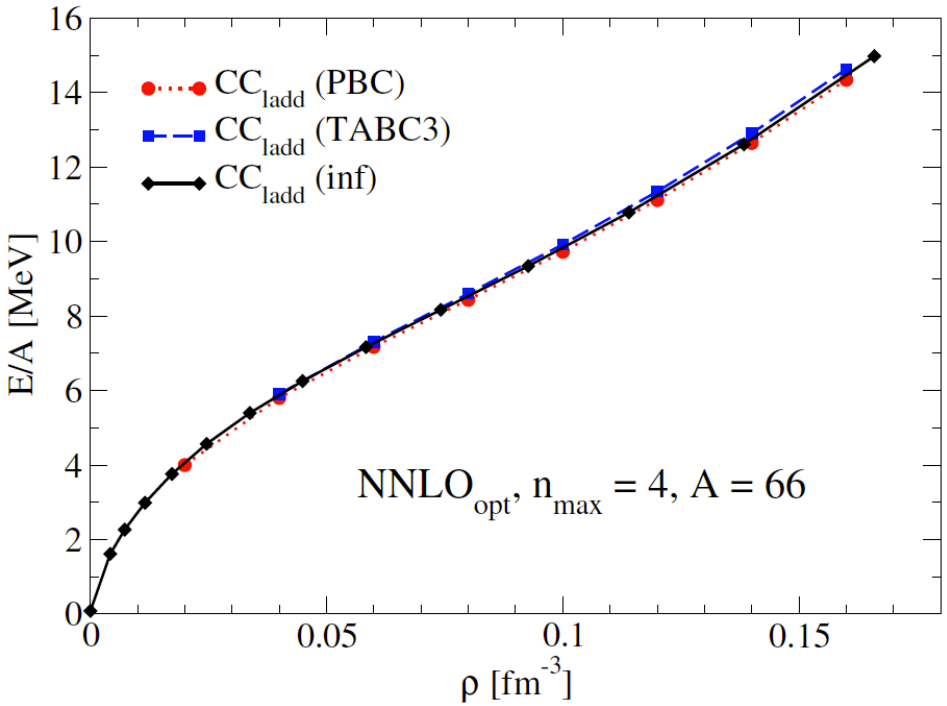
[Weinberg; van Kolck; Epelbaum *et al*.; Entem & Machleidt; …]



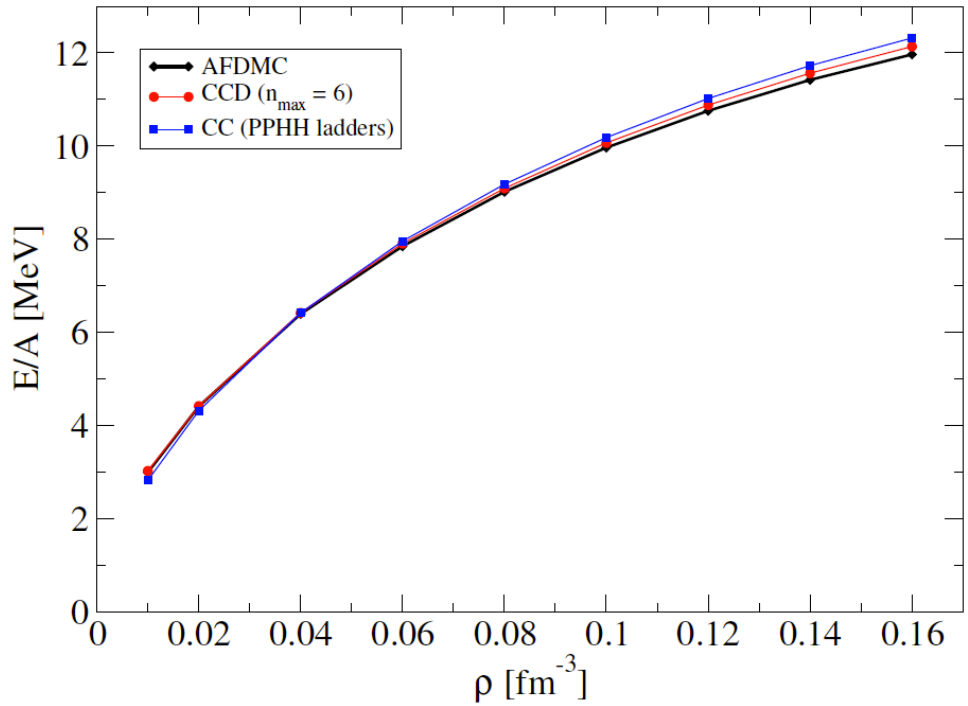
- developing higher orders and higher rank (3NF, 4NF) [Epelbaum 2006; Bernard et al 2007; Krebs et al 2012; Hebeler et al 2015; …]
- implemented in continuum and on lattice [Borasoy et al 2007]
- local / non-local formulations [Gezerlis et al 2013]
- propagation of uncertainties on horizon [Navarro Perez 2014]
- different optimization protocols [Ekström et al 2013]

Much improved understanding and handling via renormalization group transformations [Bogner et al 2003; Bogner et al 2007]

Benchmark calculations of neutron matter



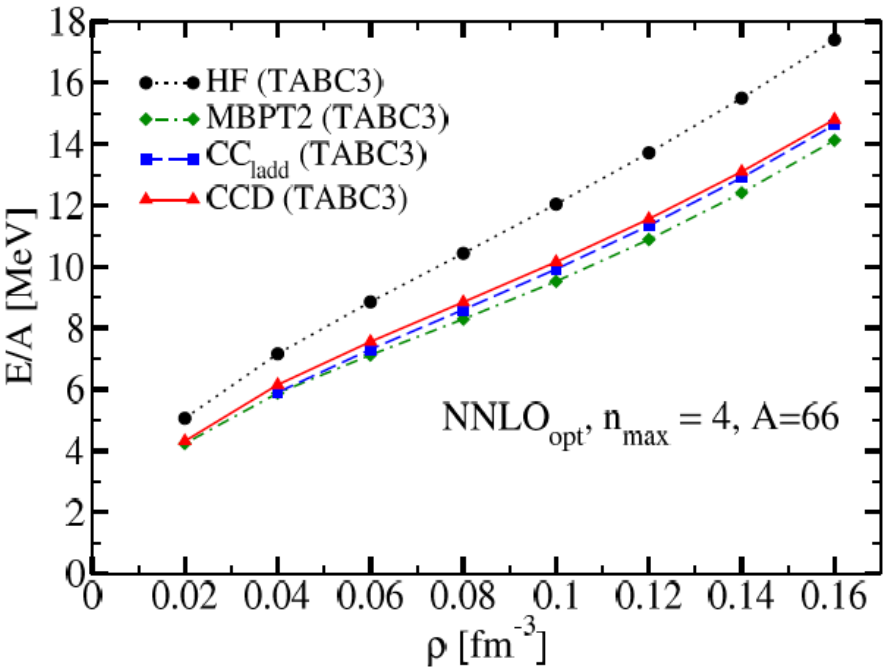
Comparison with continuum coupled-cluster method [Baardsen *et al.*, PRC (2013)]



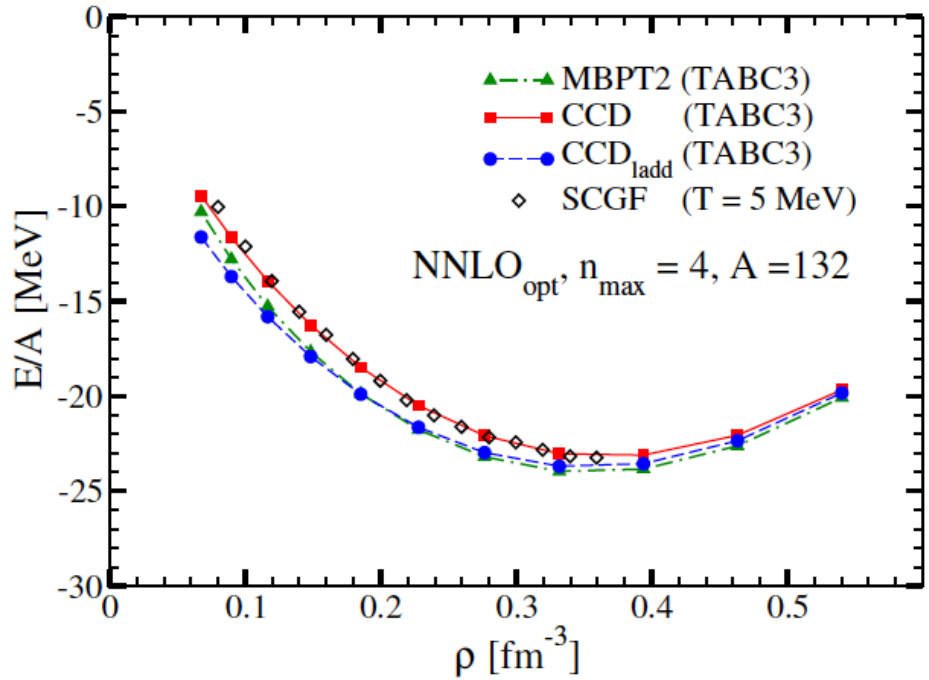
Comparison with auxiliary field diffusion Monte Carlo and Minnesota potential

Role of particle-hole excitations in nucleonic matter

Pure neutron matter (NN-only)



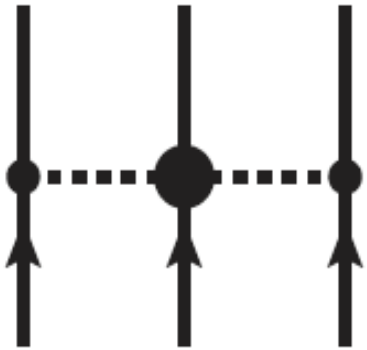
Symmetric nuclear matter (NN-only)



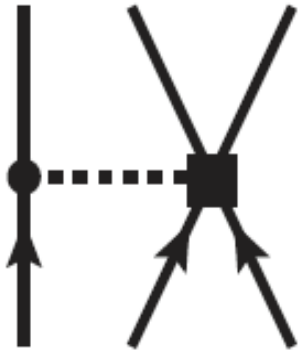
- Particle-hole and non-linear terms in CCD are small in pure neutron matter.
- MBPT2/CCD$_{ladd}$/CCD results agree within 500keV/A. Indicates that PNM is perturbative
- Particle-hole and non-linear terms play a larger role in symmetric nuclear matter.
- CCD$_{ladd}$ and CCD results differ by up to 1.5MeV/A around saturation density.

Three nucleon force (3NF) and regulator dependence

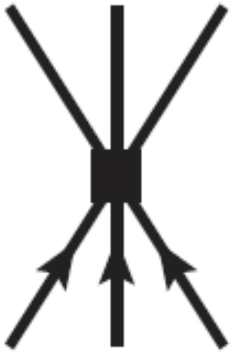
van Kolck, Phys. Rev. C 49, 2934 (1994); Epelbaum et al., Phys. Rev. C 66, 064001 (2002)



$c_{1,2,3}$



c_D



c_E

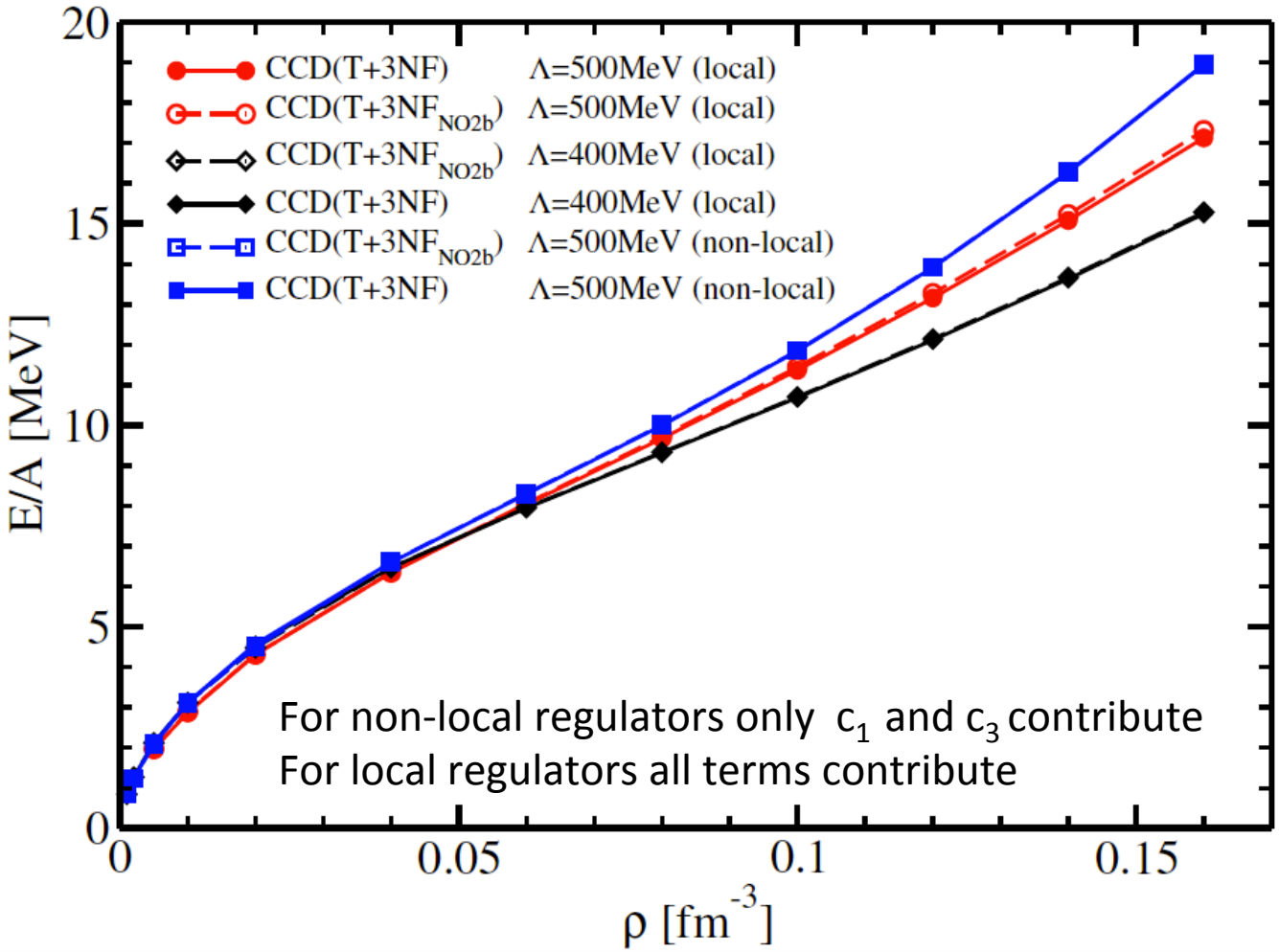
Nonlocal form of 3NF [Epelbaum et al. PRC (2002)]: Cutoff is in Jacobi momenta
Λ=500 MeV: c_D=-2, c_E=-0.791 (from A=3 binding energies)

Local form of 3NF [Navratil, Few Body Syst. (2007)]: Cutoff is in the momentum transfer

Λ=500 MeV: c_D=-0.39, c_E=-0.389 (from A=3,4 binding and ^{3}H $\tau_{1/2}$ (Gazit, Navratil, & Quaglioni)

Λ=400 MeV: c_D=-0.39, c_E=-0.27 (adjusted to ^{4}He)

Neutron matter

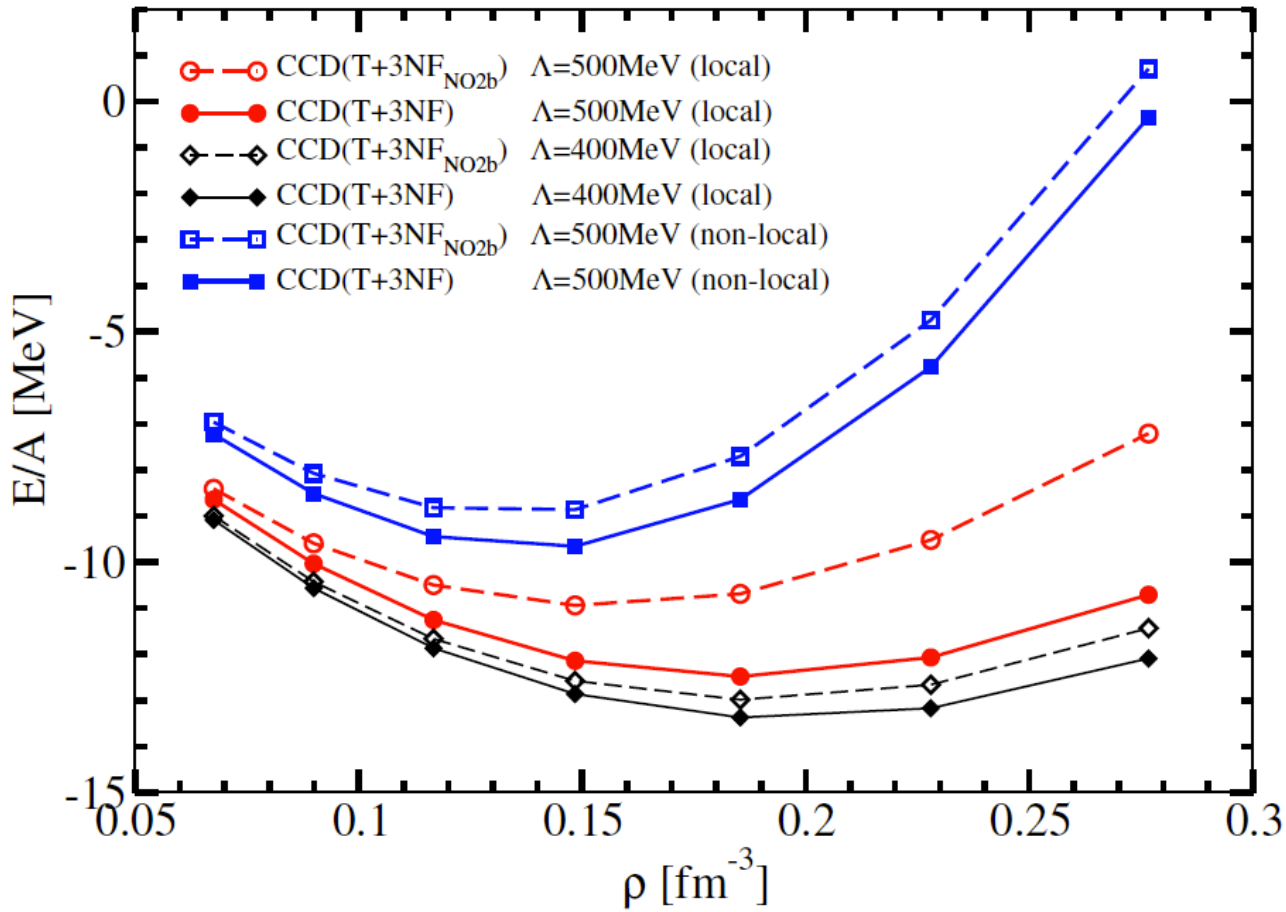


Neutron matter is perturbative (small differences between MBPT2 and coupled clusters

3NFs act repulsively in neutron matter and $NNLO_{opt}$

Error bands from variation of cutoffs and level of sophistication in treating 3NFs

Symmetric nuclear matter

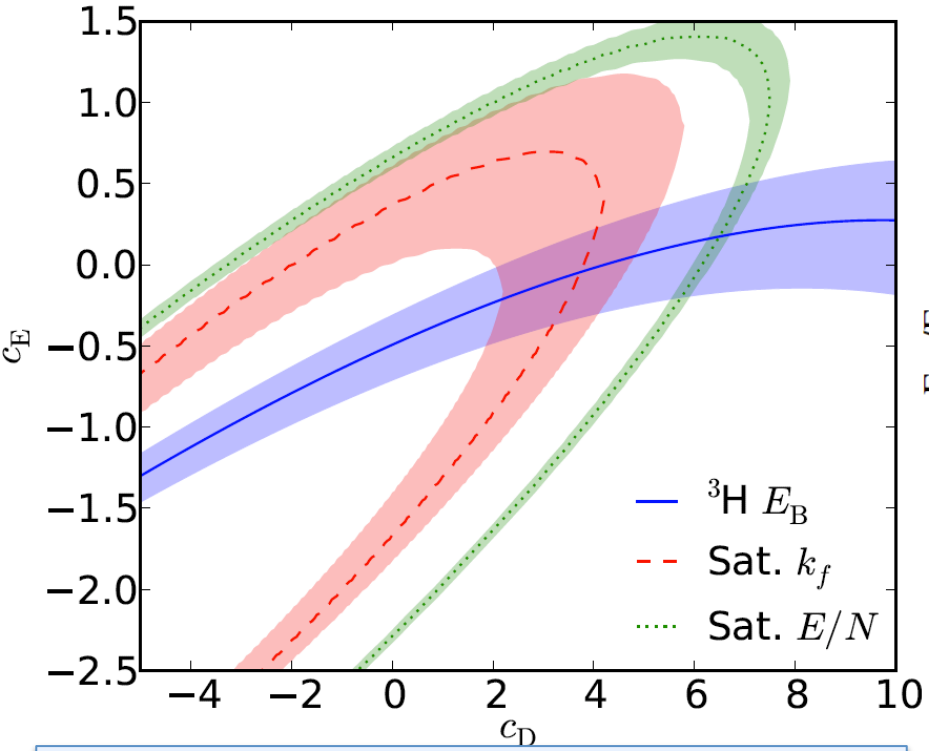


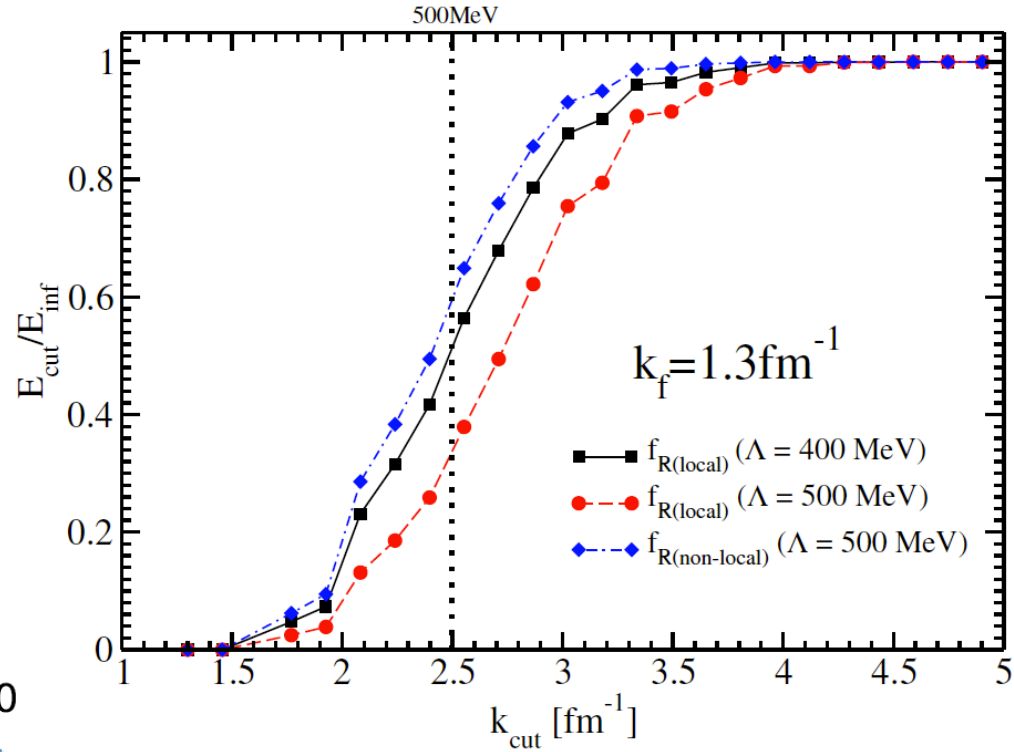
Nuclear matter is not perturbative (larger differences between MBPT2 and coupled clusters)

3NFs act repulsively in nuclear matter and NNLO$_{opt}$

☹ Regularization scheme dependence of 3NF; sensitivity to sophistication in treatment of 3NFs

Understanding the 3NF at NNLO





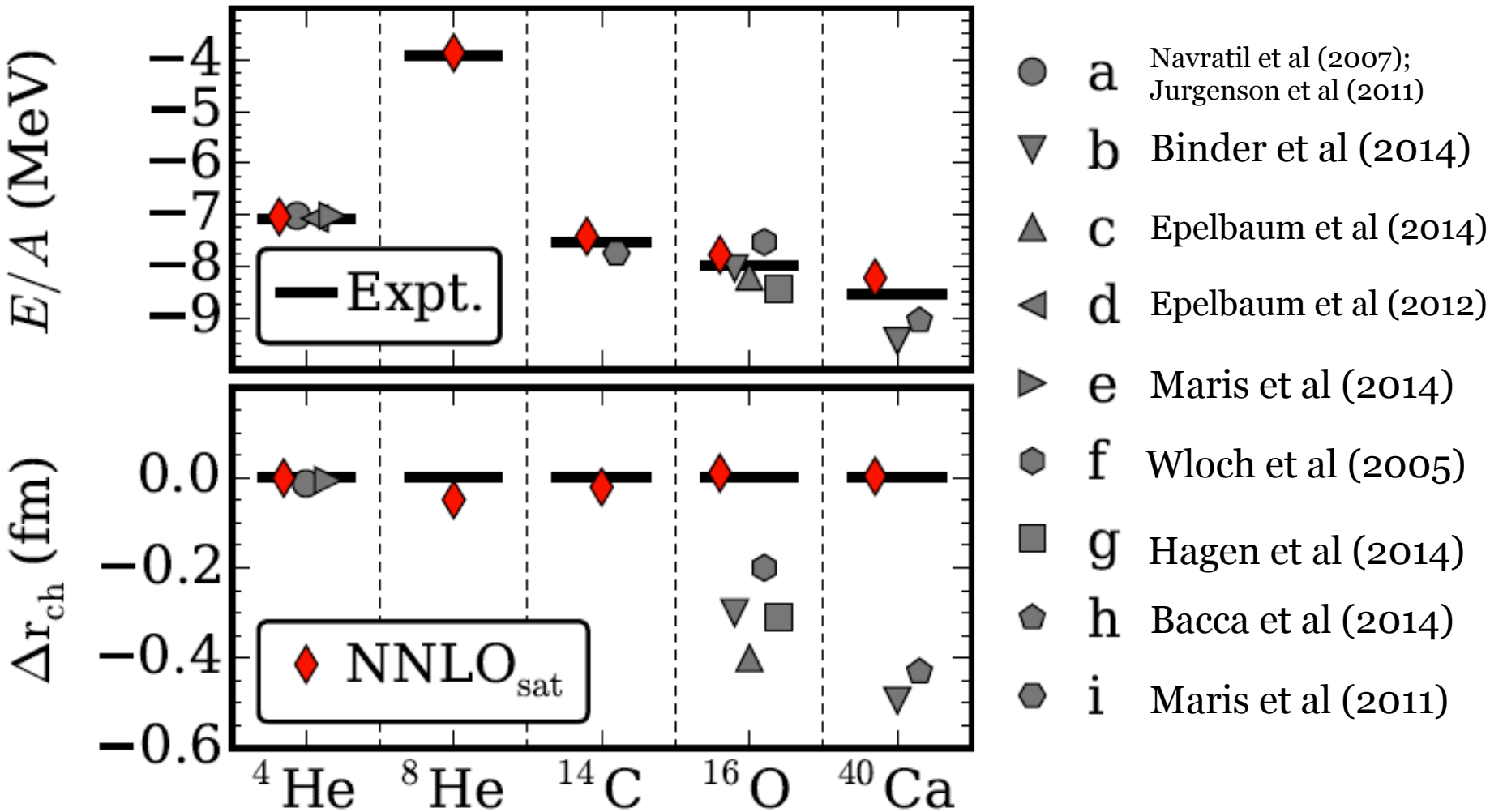
5% error bands for saturation k_f, E/N and binding energy of ^{3}H

☹ Variation of c_D and c_E not sufficient to simultaneously bind light nuclei and nuclear matter

Cutoff dependent fraction of residual 3NF contribution to MBPT2 energy per particle in SNM around saturation density.

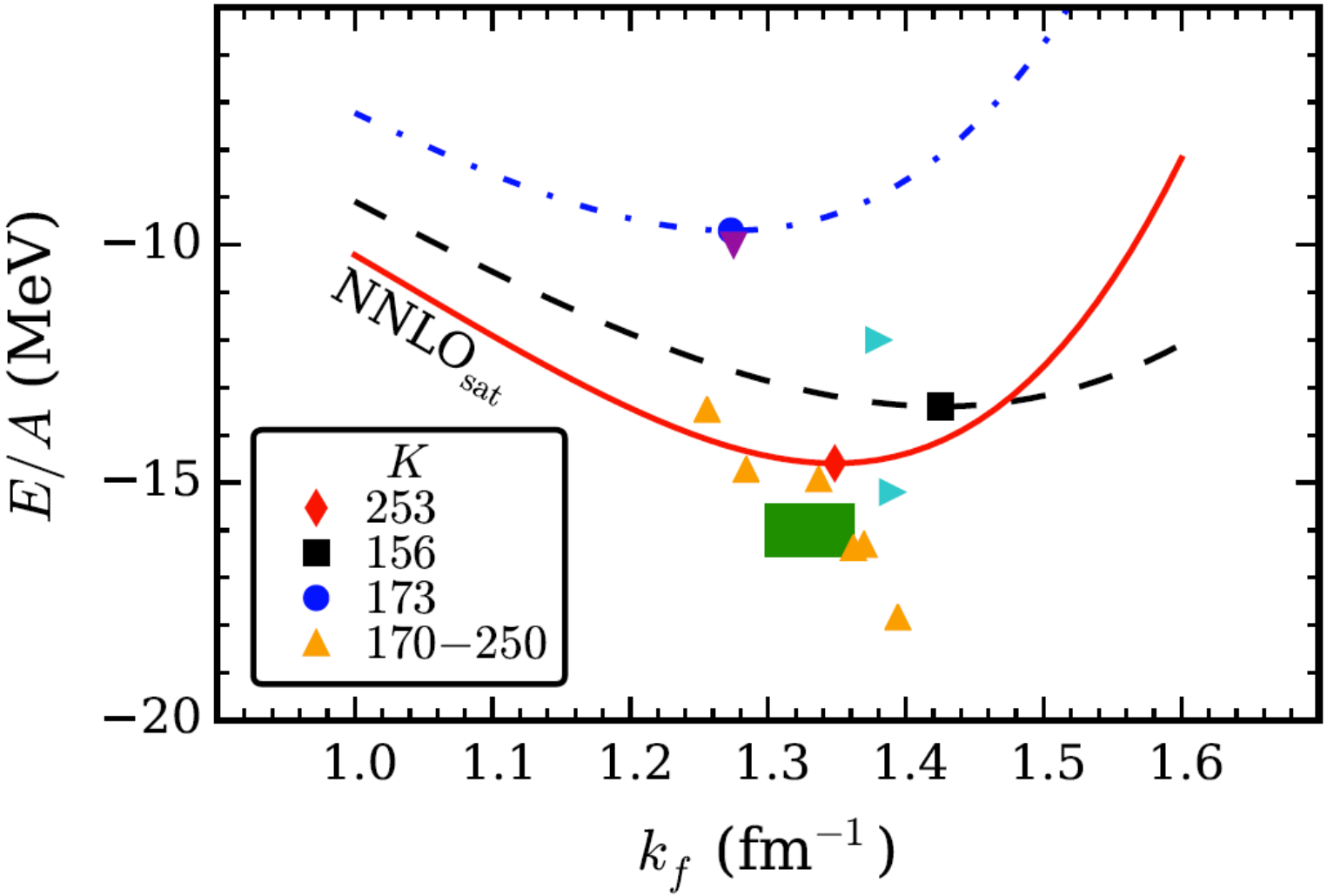
Local regulators converge slower than non-local regulators

Accurate nuclear binding energies and radii from a chiral interaction



Our solution: simultaneous optimization of NN and 3NFs with input from selected nuclei up to A ~ 25 ($NNLO_{sat}$). A. Ekström *et al*, Phys. Rev. C **91**, 051301(R) (2015)

Nuclear matter from $NNLO_{sat}$



Nuclear matter saturation curves for $NNLO_{sat}$ and other interactions.
Hagen et al (2014); Carbone et al (2013); Coraggio et al 2014;
Hebeler *et al* PRC 2011.