Ground state and dynamical properties of many–body systems by non conventional QMC algorithms

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Adelchi Fabrocini's Day, Elba - 1 July, 2016

Outline & Acknowledgements

1. Dynamical Response of Quantum many–body systems using Integral Transform techniques (and Monte Carlo)
2. Monte Carlo simulations for non-local χ-EFT interactions

Collaborators:

- Francesco Pederiva - UNITN (1,2)
- Giuseppina Orlandini - UNITN (1)
- Stefano Gandolfi and Joe Carlson - LANL (1)
- Abhishek Mukherjee - ECT* (2)

Dynamical Response of Quantum many–body systems using Integral Transform techniques

- Integral Transforms
- Dynamical Response Function
- Monte Carlo and Laplace transform
- A new transform
- Applications and perspectives

Integral Transform Techniques

An Integral Transform maps the original problem in a new domain where it's simpler to solve it

$$T(y) = \int_X K(x,y)\, S(x)\, dx$$

- Accessible object → $T(y)$
- Object of interest → $S(x)$

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$$T(y) = \int_X K(x,y)\, S(x)\, dx$$

- Accessible object
- Object of interest

The solution is then mapped back using the *inverse transform*.

PROBLEM

The inverse transform is a so–called Ill-Posed Problem!

Our object of interest: Dynamics of Quantum systems

$$\mathcal{R}(\omega) = \sum_\nu |\langle\Psi_\nu|\hat{O}|\Psi_0\rangle|^2 \delta\left(\omega - (E_\nu - E_0)\right)$$
$$= \langle\Psi_0|\hat{O}^\dagger \delta\left(\omega - (\hat{H} - E_0)\right)\hat{O}|\Psi_0\rangle$$

Or considering an IT [Efros,Leidemann,Orlandini,Phys.Lett.B 338,130]:

$$\Phi(\sigma) = \int K(\sigma,\omega)\mathcal{R}(\omega)d\omega$$

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$$\Phi(\sigma) = \int K(\sigma,\omega)\mathcal{R}(\omega) d\omega$$

A good kernel K should be one such that:

- the transform $\Phi(\sigma)$ is easy to calculate (in QMC)
- the inversion of the transform can be made stable

Integral kernels - Laplace

In QMC methods we routinely use the imaginary-time propagator

$$e^{-\tau \hat{H}}|\phi\rangle = \sum_{n=0}^{\infty} e^{-\tau E_n} \langle \Psi_n|\phi\rangle|\Psi_n\rangle \xrightarrow{\tau\to\infty} e^{-\tau E_0}\langle \Psi_0|\phi\rangle|\Psi_0\rangle$$

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In this framework it is natural to consider the Laplace kernel:

$$K(\sigma,\omega) = e^{-\sigma\omega}$$

The transform becomes an imaginary-time correlation function:

$$\Phi(\sigma) = \langle\Psi_0|\hat{O}^\dagger e^{-\sigma\hat{H}}\hat{O}|\Psi_0\rangle = \langle\Psi_0|\hat{O}^\dagger(0)\hat{O}(\sigma)|\Psi_0\rangle.$$

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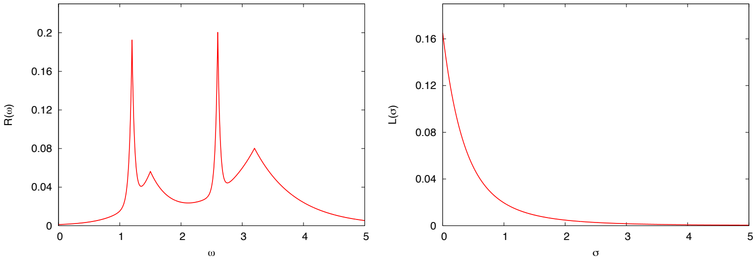
$$L(\sigma) = \int K(\sigma,\omega)R(\omega)d\omega = \int_0^\infty e^{-\sigma\omega}\, R(\omega)d\omega$$



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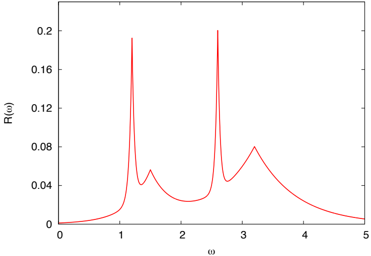

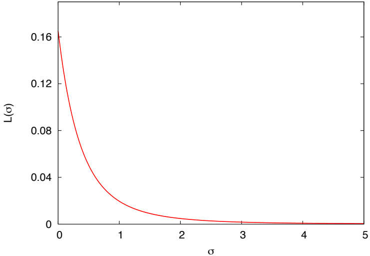

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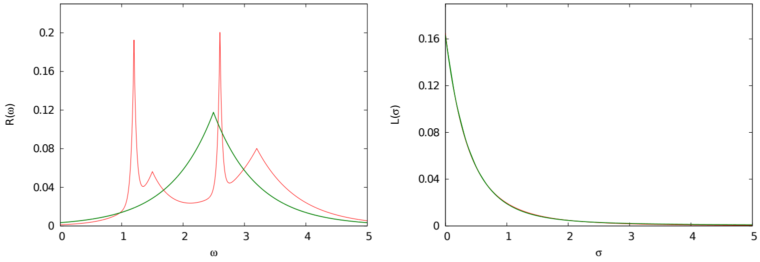

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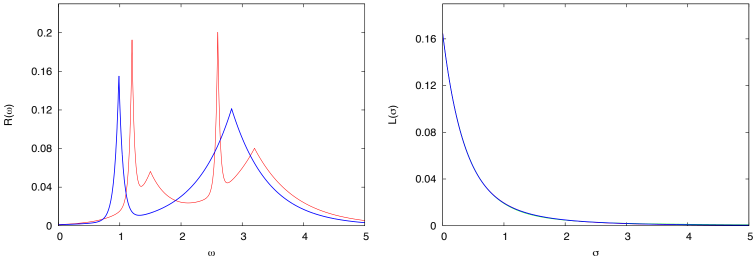

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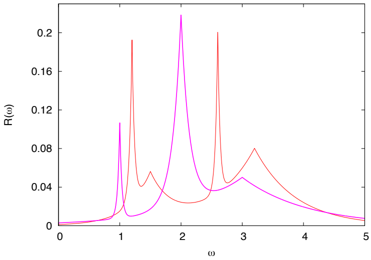

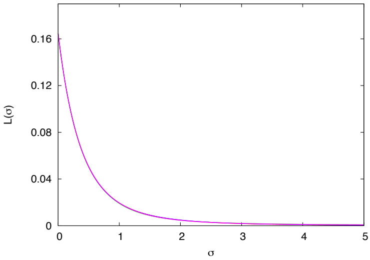

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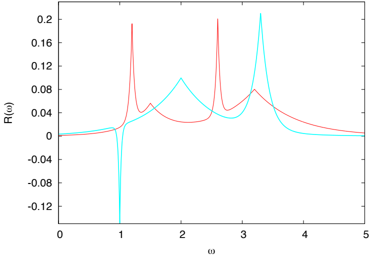

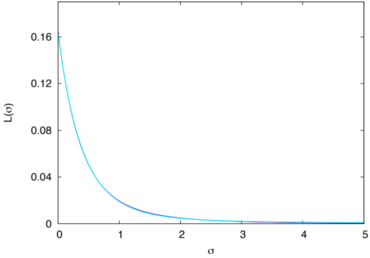

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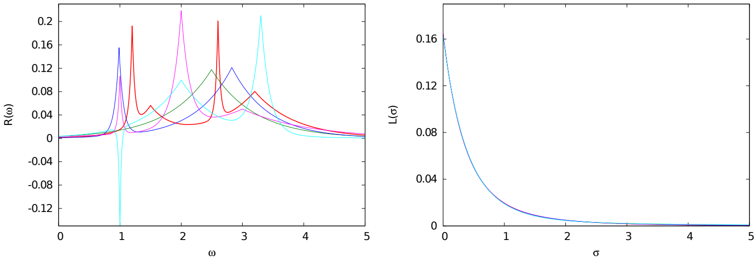

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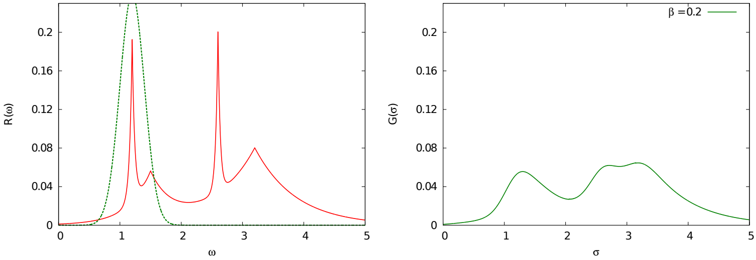
Integral kernels - Gaussian

$$G(\sigma,\beta) = \int K(\sigma,\omega,\beta)R(\omega)d\omega = \int_0^\infty e^{-\frac{(\sigma-\omega)^2}{2\beta}}\,R(\omega)d\omega$$

- We have now one more parameter: β.



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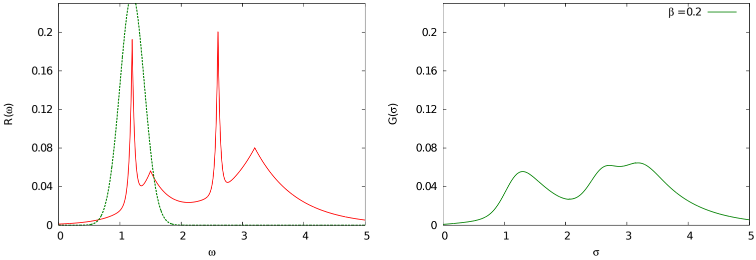

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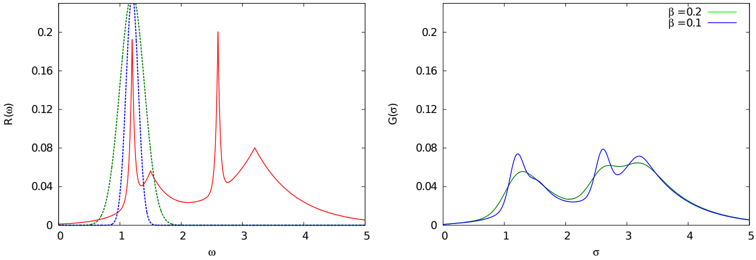

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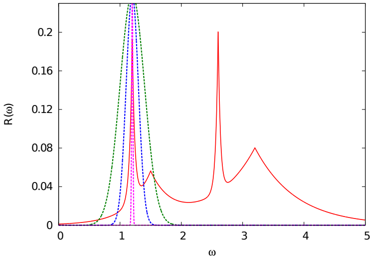

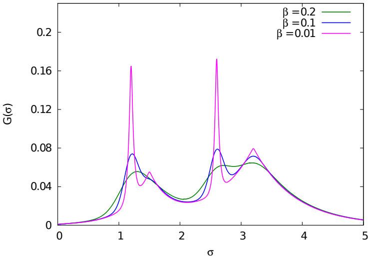

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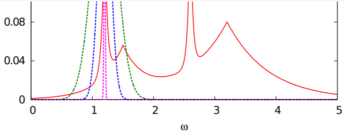

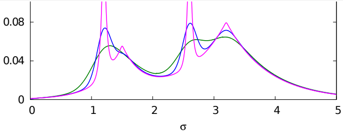

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- we can't use Gaussian (or Lorentzian) in QMC

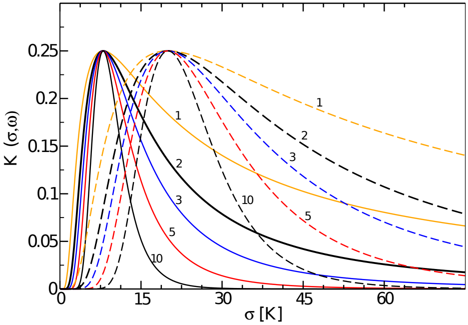
- but we have found a viable kernel

The transform $G(\sigma)$ is a smoothened version of the original signal!

We now want to build an integral kernel which can be calculated in QMC methods and that has the desired "bell–shaped" form.

$$K(\sigma,\omega,N) = \frac{1}{\sigma}\left(e^{-\ln(2)\frac{\omega}{\sigma}} - e^{-2\ln(2)\frac{\omega}{\sigma}}\right)^N = \frac{1}{\sigma}\sum_{k=0}^{N}\binom{N}{k}(-)^k e^{-\ln(2)(N+k)\frac{\omega}{\sigma}}$$

As $N \to \infty$ the kernel width becomes smaller and smaller



Recap of the idea

- take Laplace transform:

$$L(\tau) = \int K_L(\omega, \tau) R(\omega) d\omega$$

- build the new transform:

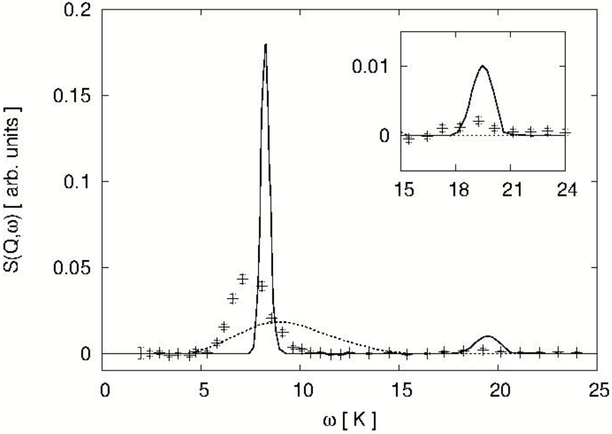
$$\Phi(\sigma, N) = \sum_j^N c_{j,N} \, L\left(\frac{a_{j,N}}{\tau}\right)$$
$$= \int K_{new}(\omega, \sigma, N) R(\omega) d\omega$$

- invert the final transform:

$$R(\omega) = \int K_{new}^{-1}(\omega, \sigma, N) \Phi(\sigma, N) d\sigma$$
$$= \int K_L^{-1}(\omega, \tau) L(\tau) d\tau$$

Density response of superfluid He^4

[A. R., F. Pederiva and G. Orlandini, PRB 88,094302 (2013)]



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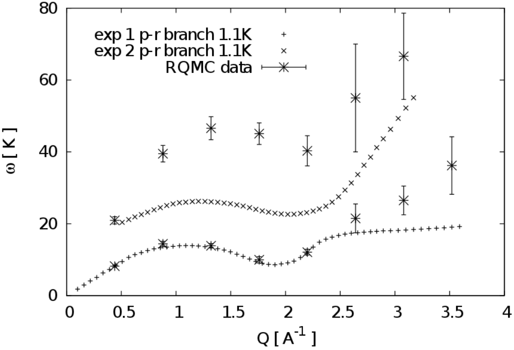


Conclusions

Pro

- may control stability of the inversion by tuning kernel function
- we need just imaginary-time correlation functions

Con

- for high accuracy, extremely long imaginary-time intervals have to be considered (computationally heavy)
- the inversion procedure can still introduce uncontrollable errors
  $\longrightarrow$ try with different Kernels (e.g. Gaussian [see next part])
  $\longrightarrow$ check different inversion schemes (e.g. GIFT [E.Vitali et al.])

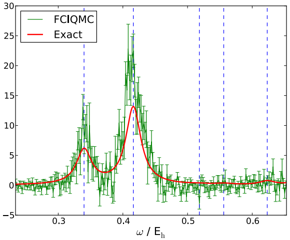
Future perspectives

Inversion of the IT remains an Ill–Posed problem, can we avoid it?

ground–state MC: $e^{-\tau\hat{H}}|\Phi_0\rangle \xrightarrow{\tau\to\infty} c_0|\Psi_0\rangle$

excited–state MC: $e^{-\tau\left(\hat{H}-E_k\right)^2}|\Phi_0\rangle \xrightarrow{\tau\to\infty} \sum_i \delta(E_i - E_k)c_i|\Psi_i\rangle \propto|\Psi_k\rangle$

$$K(E_k,\hat{H},N)|\Phi_0\rangle \xrightarrow{N\to\infty} \sum_i \delta(E_i - E_k)\tilde{c}_i|\Psi_i\rangle \propto|\Psi_k\rangle$$



Expand gaussian for $\tau \to 0$:

$$e^{-\tau\left(\hat{H}-E_k\right)^2} \approx \mathbf{1} - \tau\left(\hat{H} - E_k\right)^2$$

Booth & Chan, J.C.P. 137,191102 (2012)

Monte Carlo simulations for χ-EFT interactions

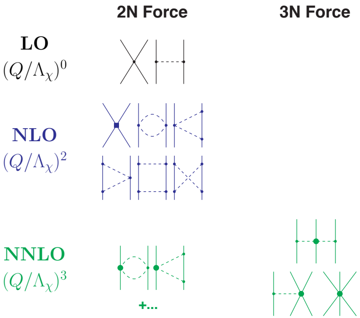
- Chiral-EFT interactions
- Dealing with non–localities with QMC
- Applications to neutron matter

Chiral Effective Field Theory (χ-EFT) interactions

- pions interact weakly at small energies (Goldstone bosons)

low-scales Q, m_π high-scales m_ρ,$\Lambda_\chi = m_\Delta - m_N$

- expand the interaction in powers of Q/Λ_χ, m_π/Λ_χ



- short range contact–interaction + pions
- many–body forces treated in a systematic way

R. Machleidt, D. R. Entem,
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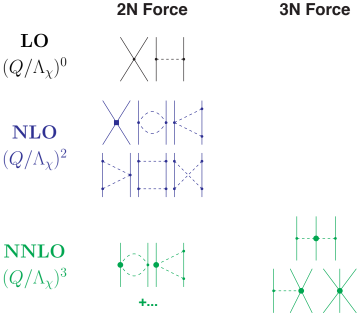

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- short range contact–interaction + pions
- many–body forces treated in a systematic way
- non–local in coordinate–space (≥NLO)

$$V(x, y) \neq V(x)\delta(x - y)$$

Locality is needed for conventional QMC

Gezerlis et al., PRL 111, 032501 (2013)

Monte Carlo methods

Use a projection operator to filter the ground–state

$$P[\hat{H}]|\Psi_n\rangle = |\Psi_{n+1}\rangle \quad | \quad \lim_{n\to\infty} P[\hat{H}]^n|\Phi_T\rangle = |0\rangle$$

$$\text{eg.} \quad P_a[\hat{H}] = 1 - \Delta\tau\hat{H} \quad \text{or} \quad P_b[\hat{H}] = e^{-\Delta\tau\hat{H}}$$

the projection is performed stochastically.

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The Standard Way

- work in coordinate–space
- for local interactions the projector factors in

$$\langle Y|e^{-\Delta\tau\hat{H}}|X\rangle = \langle Y|e^{-\Delta\tau\hat{T}}|X\rangle e^{-\Delta\tau V(X)} + O(\Delta\tau^2)$$

$$\approx G_0(Y,X)B(X)$$

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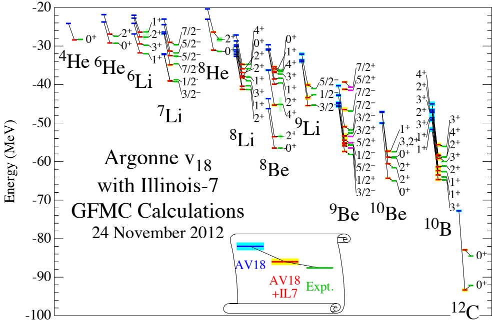

S. Pieper, R. Wiringa et. al (ANL)

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The Standard Way

- work in coordinate–space
- for non–local interactions the projector doesn't factor

$$\langle Y|e^{-\Delta\tau\hat{H}}|X\rangle = \int dZ\langle Y|e^{-\Delta\tau\hat{T}}|Z\rangle\langle Z|e^{-\Delta\tau\hat{V}}|X\rangle + O(\Delta\tau^2)$$

$$\approx \int dZ G_0(Y,Z)G_V(Z,X)$$

Finite basis version

$$\hat{H} = \sum_{a}^{\Omega} \epsilon_a \hat{a}_a^\dagger \hat{a}_a + \frac{1}{2} \sum_{ijkl}^{\Omega} V_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l + \dots$$

- Direct Diagonalization possible only for small systems
- A general V_{ijkl} leads to non–local interactions

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The Finite Basis Way

- work in occupation number basis: $|\mathbf{n}\rangle = |\dots 01100010 \dots\rangle$
- for any interaction the projector can be written as

$$\langle \mathbf{m}|\hat{P}|\mathbf{n}\rangle = \left(\frac{\langle \mathbf{m}|\hat{P}|\mathbf{n}\rangle}{\sum_{\mathbf{m}} \langle \mathbf{m}|\hat{P}|\mathbf{n}\rangle} \right) \left(\sum_{\mathbf{m}} \langle \mathbf{m}|\hat{P}|\mathbf{n}\rangle \right) = p(\mathbf{m},\mathbf{n}) w(\mathbf{n})$$

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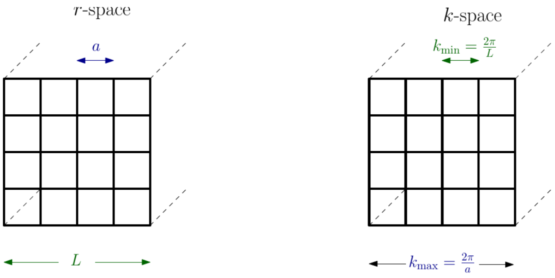
- We can use Coupled–Cluster theory to circumvent the sign–problem

Single–particle basis for bulk systems



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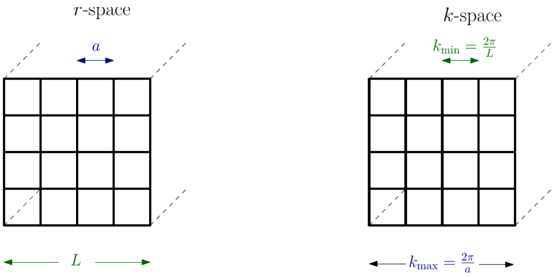

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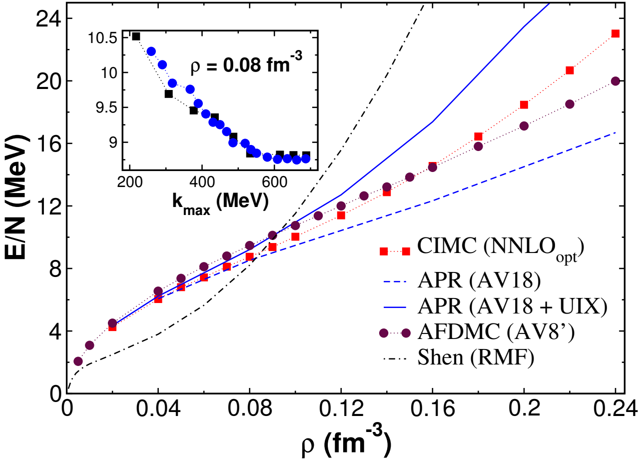
Coulomb gas $\longrightarrow$ good agreement with R–space QMC calculations

[A. R., A. Mukherjee and F. Pederiva, PRB 88,115138 (2013)]

Neutron Matter with χ-EFT interactions at N2LO

Equation of State



[A. R., A. Mukherjee and F. Pederiva, PRL 112, 221103 (2014)]

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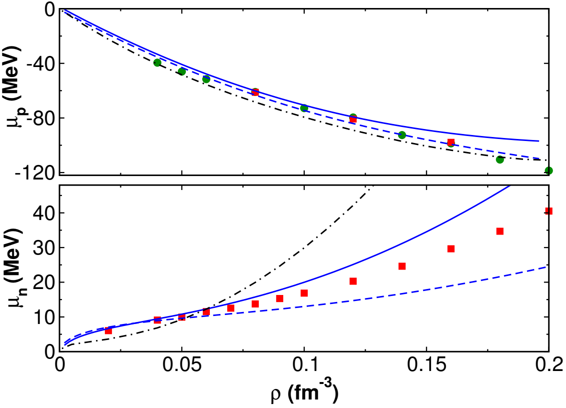
Nucleon chemical potential



[A. R., A. Mukherjee and F. Pederiva, PRL 112, 221103 (2014)]

Conclusions

Summary:

- we have developed a MC method that works for general interactions providing rigourus upper–bounds on energy
- the use of Coupled Cluster Wave–functions serves a dual pourpose:
  - extremely good guiding wave–function
  - provides variational energies for CC solutions

Current & Future work:

- extension to finite systems
- solving sign-problem with cancellation (à la FCI-QMC)
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Thanks for your attention

Wave–functions for Importance Sampling

A very accurate way to account for correlations in a generic Fock–space is the Coupled Cluster ansatz:

$$|\Psi_T\rangle = e^{-\hat{T}}|\Phi_{HF}\rangle \quad \text{with} \quad \hat{T} = \hat{T}_1 + \hat{T}_2 + \dots$$

Here we will restrict to CCD case: $\hat{T} = \hat{T}_2 = \frac{1}{2}\sum_{ij,ab} t_{ij}^{ab}\hat{a}_a^\dagger\hat{a}_b^\dagger\hat{a}_j\hat{a}_i$.

Is the CCD wave–function even quick to evaluate in SD space?

We need to calculate

$$\Phi^m_{\mathrm{CCD}}\left(\begin{smallmatrix} p_1 p_2 \cdots p_m \\ h_1 h_2 \cdots h_m \end{smallmatrix}\right) = \Phi_{\mathrm{CCD}}(\mathbf{n}) \quad \text{for} \quad |\mathbf{n}\rangle = a^\dagger_{p_1}\dots a^\dagger_{p_m} a_{h_1}\dots a_{h_m}|\Phi_{\mathrm{HF}}\rangle$$

It turns out that one can write a **recursive formula** ([arXiv:1304.1549])

$$\Phi^m_{\mathrm{CCD}}\left(\begin{smallmatrix} \cdots \\ \cdots \end{smallmatrix}\right) = \sum_{\gamma=2}^{m}\sum_{\mu<\nu}^{m}(-)^{\gamma+\mu+\nu} t^{p_\mu p_\nu}_{h_1 h_\gamma}\Phi^{m-2}_{\mathrm{CCD}}\left(\begin{smallmatrix} \cdots \\ \cdots \end{smallmatrix}\right)$$

Singular Value Decomposition (SVD)

We can make a discretization of the Integral transform

$$g(x) = \int_a^b K(x,y) f(y) dy \quad \longrightarrow \quad g_i = \sum_k^N \alpha_k K_{ik} f_k \quad i \in [1, N]$$

$$g_i \equiv g(x_i) \quad K_{ik} \equiv K(x_i, y_k) \quad f_k \equiv f(y_k)$$

The SVD of the matrix K is a factorization of the form

$$K = U \Sigma V^T \quad \text{with} \quad U, V, \Sigma \in \mathbb{R}^{NxN}$$

with U, V orthogonal and $\Sigma = diag[\sigma_1, \ldots, \sigma_N]$.

The columns $\bar{u}_j$ of U and $\bar{v}_j$ of V can be regarded as orthonormal basis vectors of $\mathbb{R}^N$ and the following holds

$$K \bar{v}_j = \sigma_j \bar{u}_j \quad K^T \bar{u}_j = \sigma_j \bar{v}_j$$

Singular Value Decomposition (SVD) II

In terms of the SVD of the matrix K the direct and inverse problems can be rewritten as

$$\bar{g} = K\bar{f} = \sum_{j}^{N} \sigma_j (\bar{v}_j^T \bar{f}) \bar{u}_j \qquad \bar{f} = K^{-1}\bar{g} = \sum_{j}^{N} \frac{\bar{u}_j^T \bar{g}}{\sigma_j} \bar{v}_j$$

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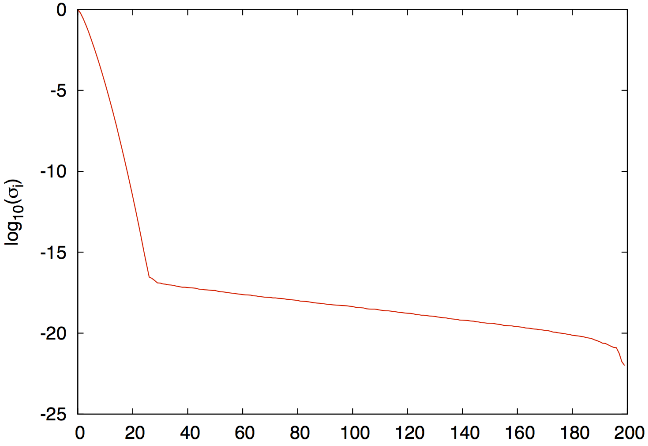
If the matrix K is the result of discretization of a Fredholm Integral equation of the 1st kind the following basic properties holds

- the singular values σ_i decay fast towards zero
- the singular vectors $\bar{u}_i$,$\bar{v}_i$ have increasing frequencies

We can use the decay rate of singular values to define a sort of *degree of* $ill - posedness$

Singular Value Spectrum



Regularization techniques

The idea is to approximate our original ill-posed problem with a well-posed one, constraining the solution with known features.

In most approaches we have minimization problems of the form

$$\min_{\bar{f}} \quad D\left[K\bar{f}, \bar{g}\right] + \alpha L\left[\bar{f}\right]$$

where

- D is a likelihood function (eg. Chi-squared, euclidean norm)
- L is a penalty functional that enforces eg. smoothness
- α is the regularization parameter

Regularization techniques: some examples

Regularized Least Squared (Tikhonov)

$$\min_{\bar{f}} \; \|K\bar{f} - \bar{g}\|^2 + \alpha\|\Gamma\bar{f}\|^2$$

where the Tikhonov matrix Γ can be the identity I or a discrete version of a derivative operator D_1,D_2.

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Cross-Entropy Minimization

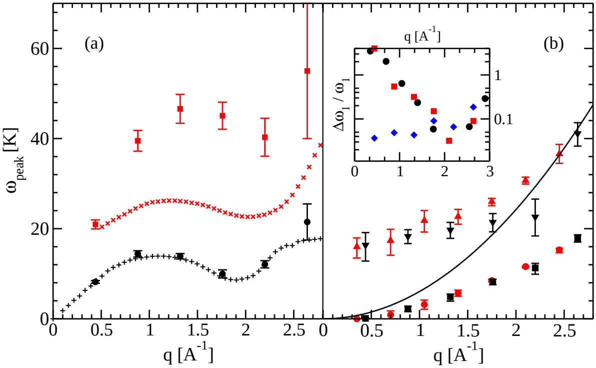
$$\min_{\bar{f}} \; KL\left[K\bar{f}, \bar{g}\right] + \alpha KL\left[\bar{f}, \bar{f}_0\right]$$

where KL is the Kullback-Leibler distance

$$KL\left[\bar{a}, \bar{b}\right] = \sum_n a_n log(a_n/b_n) + b_n - a_n$$

and $\bar{f}_0$ is some prior estimate of $\bar{f}$ (usually a positive constant)

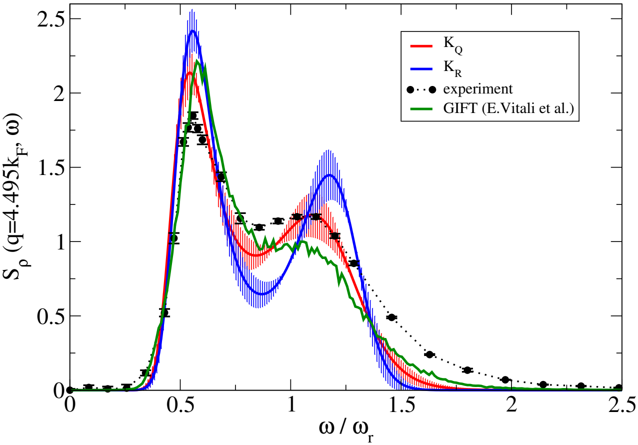
Density response of He4



Density response of Unitary Fermi Gas

in collaboration with S.Gandolfi and J. Carlson(LANL)

PRELIMINARY RESULTS



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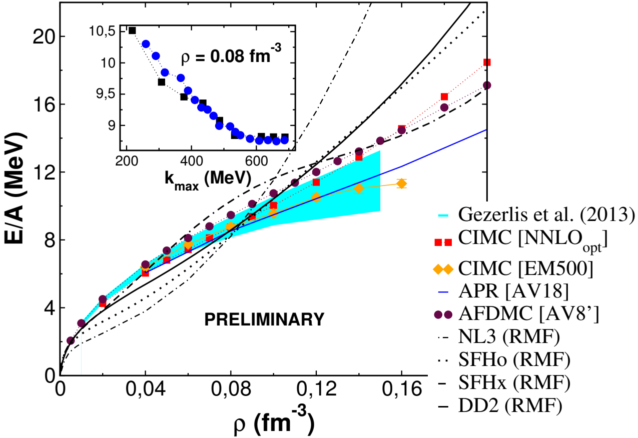
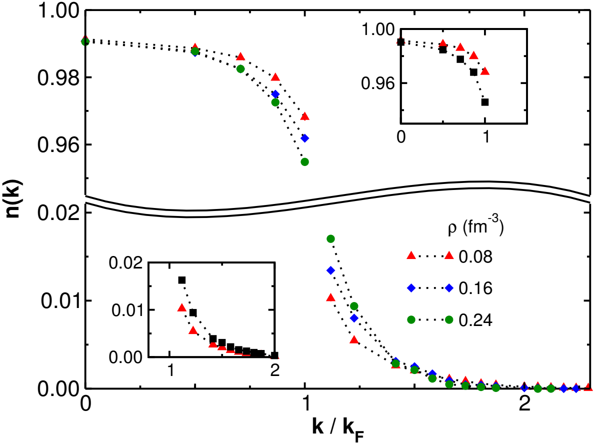


Momentum distribution



Constraining Nuclear Energy Density Functionals

Energy density functional for uniform matter:

$$\mathcal{E} = \mathcal{E}_{\rm kin} + \sum_{t=0,1} \left(C_t^\rho \rho_t^2 + C_t^\tau \rho_t \tau_t + C_t^s s_t^2 + C_t^T s_t T_t \right) .$$

- contributions from both time–even and time–odd components.
- time–even part constrained eg. by even–even nuclei
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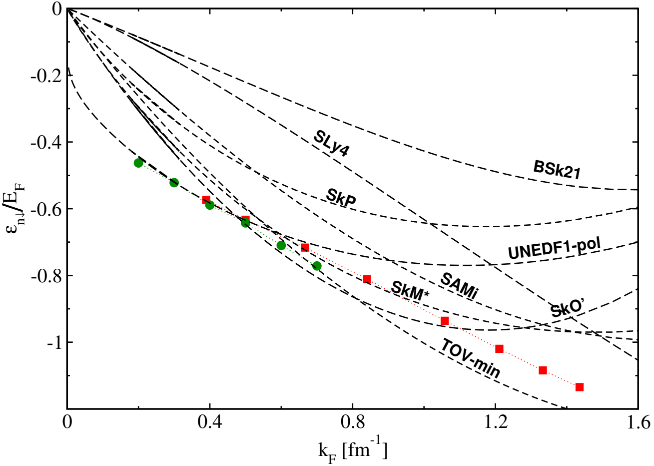
Idea: [M. M. Forbes et al. PRC 89, 041301(R) (2014)]

Calculate binding energy of an impurity in polarized neutron matter

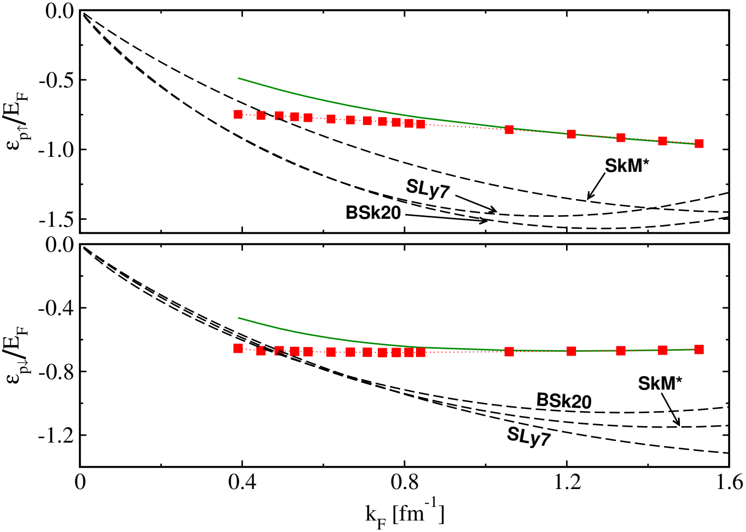
$$\varepsilon_{\tau\sigma} = \left.\frac{\partial \mathcal{E}}{\partial \rho_{\tau\sigma}}\right|_{\rho_{\tau\sigma}\to 0} \quad \rightarrow \quad \text{eg} \quad \varepsilon_{n\downarrow} \propto (C_0^s + C_1^s), (C_0^T + C_1^T)$$

The neutron polaron

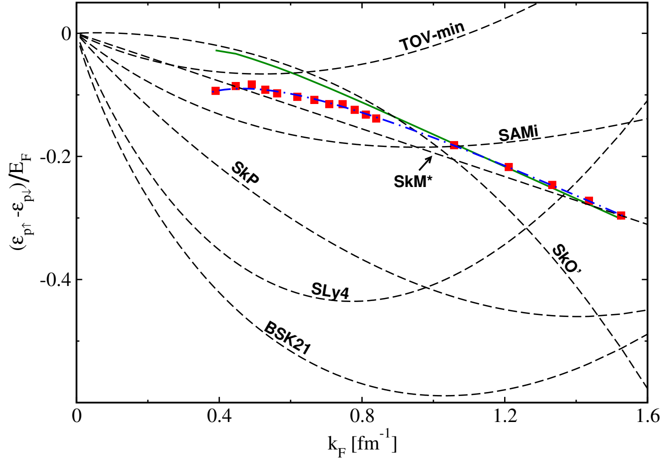


Green pts from: M. M. Forbes et al. **PRC 89, 041301(R) (2014)**

The proton polarons I

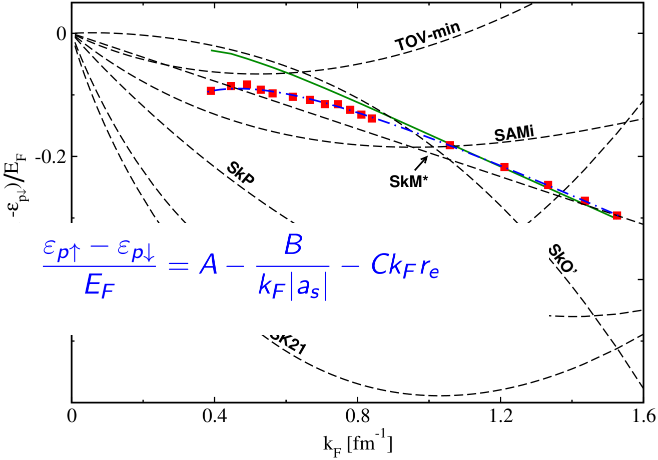


$$\frac{\varepsilon_{p\uparrow} - \varepsilon_{p\downarrow}}{E_F} = \frac{4m(C_0^s - C_1^s)}{3\pi^2\hbar^2} k_F - \frac{2m(C_0^T - C_1^T)}{5\pi^2\hbar^2} k_F^3.$$



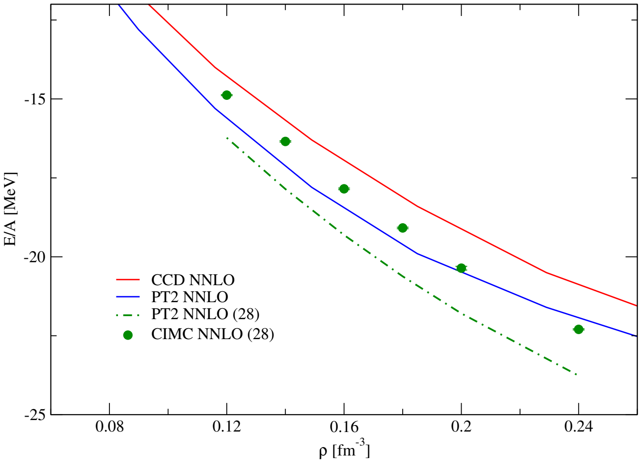
The proton polarons II

$$\frac{\varepsilon_{p\uparrow} - \varepsilon_{p\downarrow}}{E_F} = \frac{4m(C_0^s - C_1^s)}{3\pi^2\hbar^2} k_F - \frac{2m(C_0^T - C_1^T)}{5\pi^2\hbar^2} k_F^3.$$



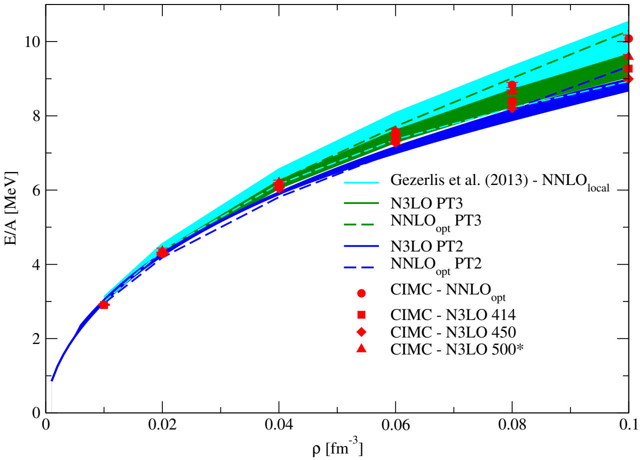
$$\frac{\varepsilon_{p\uparrow} - \varepsilon_{p\downarrow}}{E_F} = A - \frac{B}{k_F |a_s|} - C k_F r_e$$

Symmetric Nuclear Matter - finite size effects



Neutron matter with QMC & χ-EFT NN interactions

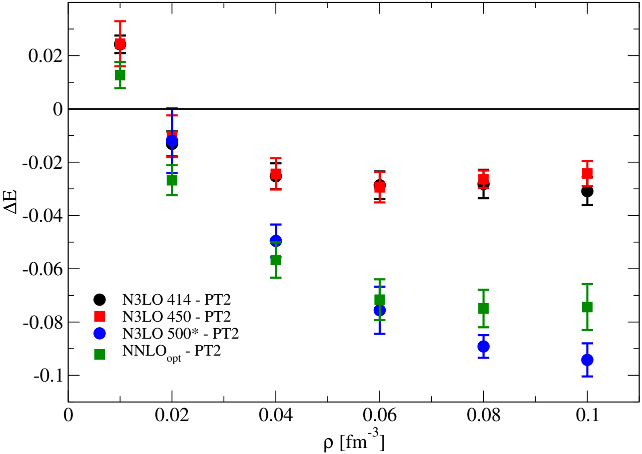
NNLO$_{opt}$ Ekström et al. (2013) N3LO 500* Entem & Machleidt (2003) N3LO 414-450 Coraggio et al. (2007)



CIMC NNLO$_{opt}$ - A.R, A. Mukherjee & F. Pederiva PRL (2014)
CIMC N3LO - A.R, E. Rrapaj, S. Reddy & J. W. Holt - in preparation

Convergence of MBPT in neutron matter

$$\Delta E \equiv \frac{E_x - E_{CIMC}}{E_{CIMC}}$$



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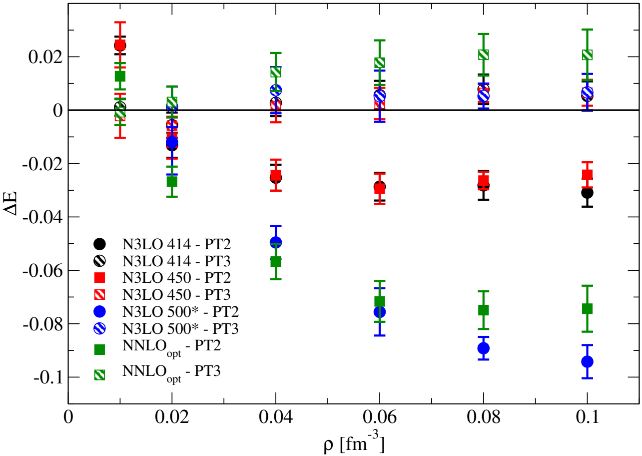

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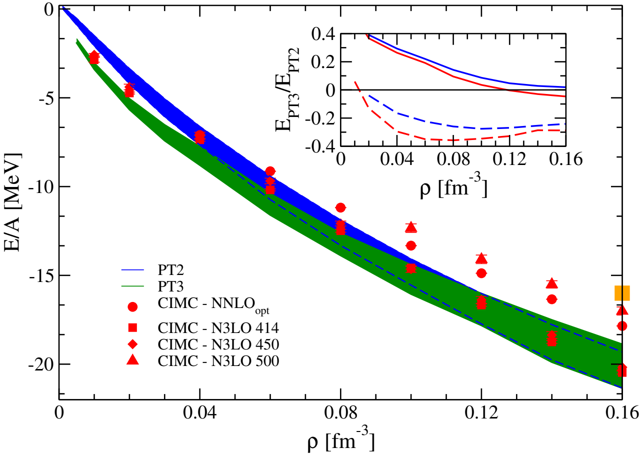

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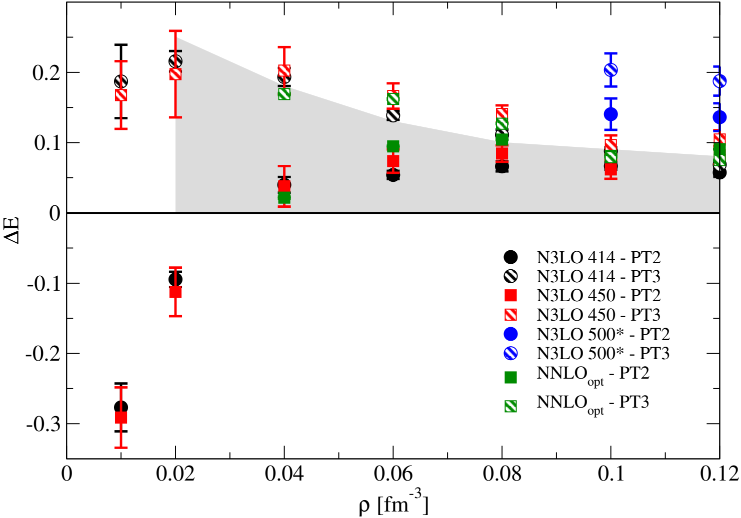

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