Nuclear Energy Density Functional from Chiral Two- and Three-Nucleon Interactions

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- Introduction: nuclear energy density functional
- Tool: (improved) density-matrix expansion
- Chiral two- and three-nucleon interactions
- Diagrammatic calculation of energy density functional
- Results for isospin-symmetric nuclear systems
- Isovector part of nuclear energy density functional
- Challenge: Consistent 2nd order calculation

Publications:

J. Holt, N. Kaiser, W. Weise, Eur. Phys. J. A47 (2011) 128; Eur. Phys. J. A48 (2012) 36.

- Nuclear energy density functional: many-body method for calculat. of medium-mass and heavy nuclei $\rightarrow$ self-consistent mean-field approx.
- Non-relativistic (parametrized) Skyrme functionals and relativistic mean-field models are widely and successfully used
- RMF: Lorentz scalar and vector mean-fields generate nuclear spin-orbit interact. (S+V fields originate from short-range NN spin-orbit, Fuchs et al.)
- Complementary approach: constrain form of a predictive energy density functional and its couplings by many-body perturbation theory and the underlying two- and three-nucleon interactions
- Switch from hard-core NN-potentials to low-momentum interactions: with V_{low-k} nuclear many-body problem becomes more perturbative
- Non-local Fock contributions to energy: approximate them by functionals expressed in terms of local densities and currents only
- Key ingredient: Density-matrix expansion
  Negele and Vautherin, Phys. Rev. C5 (1972) 1472
- Gebremariam, Bogner, Duguet, Nucl. Phys. A851 (2011) 17: used N^2LO chiral NN-potential + Skyrme $\rightarrow$ got small but systematic reduction of χ^2
- Here: Improved chiral NN-potential at N^3LO + lead. chiral 3N-interaction

Improved density-matrix expansion

- Improved density-matrix expansion via phase-space averaging:
  Gebremariam, Duguet and Bogner, Phys. Rev. C82 (2010) 14305

$$\sum_\alpha \Psi_\alpha\Big(\vec r - \frac{\vec a}{2}\Big)\Psi^\dagger_\alpha\Big(\vec r + \frac{\vec a}{2}\Big) = \frac{3\rho}{ak_f} j_1(ak_f) - \frac{a}{2k_f} j_1(ak_f)\Big[\tau - \frac{3}{5}\rho k_f^2 - \frac{1}{4}\vec\nabla^2\rho\Big] + \frac{3i}{2ak_f} j_1(ak_f)\,\vec\sigma\cdot(\vec a\times\vec J\,) + \dots$$

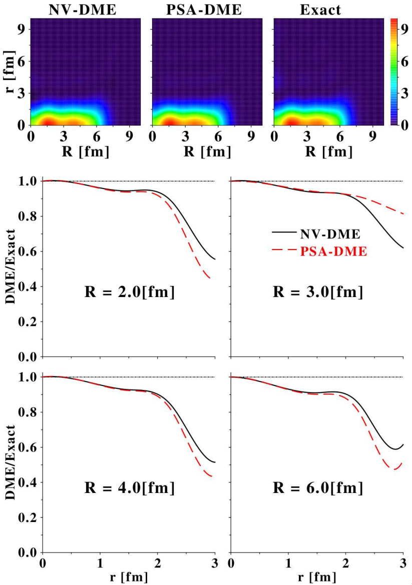
$\rho = 2k_f^3/3\pi^2$ local nucleon density, $\vec J = \sum_\alpha \Psi^\dagger_\alpha i\,\vec\sigma\times\vec\nabla\Psi_\alpha$ spin-orbit density

- Few % accuracy for Fock contrib. from central and tensor interactions
- Spin-dependent part ($\vec a\times\vec J\,$) of Negele-Vautherin DME makes 50% error
- Fourier-transform: "medium insertion" for inhomogenous nuclear system

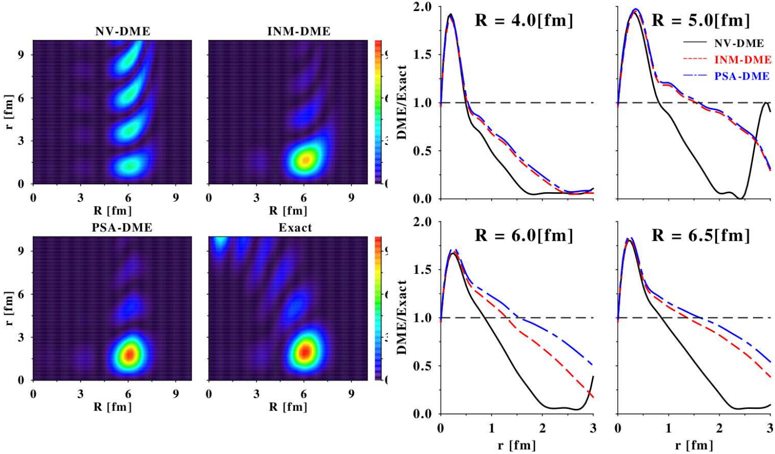
$$\Gamma(\vec p,\vec q\,) = \int d^3r\, e^{-i\vec q\cdot\vec r}\Big\{\theta(k_f - |\vec p\,|) + \frac{\pi^2}{4k_f^4}\Big[k_f\,\delta'(k_f-|\vec p\,|) - 2\delta(k_f-|\vec p\,|)\Big] \times\Big(\tau - \frac{3}{5}\rho k_f^2 - \frac{1}{4}\vec\nabla^2\rho\Big) - \frac{3\pi^2}{4k_f^4}\,\delta(k_f-|\vec p\,|)\,\vec\sigma\cdot(\vec p\times\vec J\,)\Big\}$$

generalizes step-function $\theta(k_f - |\vec p\,|)$ for infinite nuclear matter

- Comparison of density-matrix expansions: schematic central interaction



- Comparison of density-matrix expansions: tensor interaction



INM: quadrupolar deformation of local Fermi-moment. distribution neglected

Nuclear energy density functional

- Energy density functional for $N = Z$ even-even nuclei:

$$\mathcal{E}[\rho,\tau,\vec{J}\,] = \rho\bar{E}(\rho) + \left[\tau - \frac{3}{5}\rho k_f^2\right]\left[\frac{1}{2M} - \frac{k_f^2}{4M^3} + F_\tau(\rho)\right] + (\vec{\nabla}\rho)^2 F_\nabla(\rho) + \vec{\nabla}\rho\cdot\vec{J}\,F_{so}(\rho) + \vec{J}^{\,2}F_J(\rho)$$

effective nucleon mass $M^*(\rho)$, surface term, spin-orbit coupling, $\vec{J}^2$ term

- Relation to slope of single-particle potential at Fermi surface:

$$F_\tau(\rho) = \frac{1}{2k_f}\frac{\partial U(p,k_f)}{\partial p}\bigg|_{p=k_f} = -\frac{k_f}{3\pi^2}f_1(k_f)$$

i.e. same effective nucleon mass $M^*(\rho)$ as in Fermi-liquid theory

- Decomposition: for $F_d(\rho)$, factor $(\vec{\nabla}\rho)^2$ emerges directly from interaction

$$F_\nabla(\rho) = \frac{1}{4}\frac{\partial F_\tau(\rho)}{\partial\rho} + F_d(\rho)$$

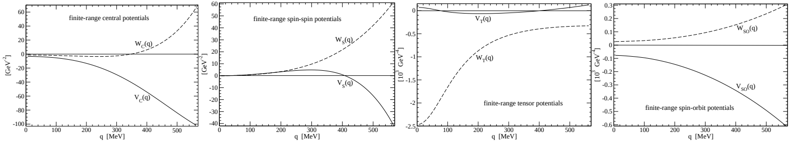
- For zero-range Skyrme force: improved density-matrix expansion and Negele-Vautherin DME give identical results (quadratic p-dependence)
- Differences expected for long-range 1π- and 2π-exchange interaction

Chiral NN and 3N interactions

- Preferred 2-body interact.: universal low-momentum NN-potential $V_{\mathrm{low-k}}$
- Partial wave matrix elements, explicit spin-isospin operators better suited
- Easier tractable substitute for $V_{\mathrm{low-k}}$: Chiral N^{3}LOW potential, $\Lambda = 414\,\mathrm{MeV}$
- Finite-range part of N^{3}LOW: one- and two-pion exchange of the form

$$\begin{aligned} V_{NN}^{(\pi)} &= V_C(q) + \vec\tau_1\cdot\vec\tau_2\, W_C(q) + \big[V_S(q) + \vec\tau_1\cdot\vec\tau_2\, W_S(q)\big]\,\vec\sigma_1\cdot\vec\sigma_2 \\ &+ \big[V_T(q) + \vec\tau_1\cdot\vec\tau_2\, W_T(q)\big]\,\vec\sigma_1\cdot\vec q\;\vec\sigma_2\cdot\vec q \\ &+ \big[V_{SO}(q) + \vec\tau_1\cdot\vec\tau_2\, W_{SO}(q)\big]\, i(\vec\sigma_1+\vec\sigma_2)\cdot(\vec q\times\vec p\,)\,, \end{aligned}$$

- dependence only on momentum transfer q, no quadratic spin-orbit comp.



- Short-range part: 24 contact terms up 4th power of momenta, C_{ST}, C_j, D_j determined in fits to NN-phase shifts and deuteron ($\rightarrow$ Machleidt's code)

Two-body contributions at 1st order

- Finite-range pieces: Hartree-Fock, employing $\Gamma\vec{p}_1, \vec{q}\,)\,\Gamma(\vec{p}_2, -\vec{q}\,)$

$$\bar{E}(\rho) = \frac{\rho}{2} V_C(0) - \frac{3\rho}{2}\int_0^1 dx\, x^2(1-x)^2(2+x)[V_C(q) + 3V_S(q) + q^2 V_T(q) + \dots]$$

$$F_\tau(\rho) = \frac{k_f}{2\pi^2}\int_0^1 dx(x - 2x^3)[V_C(q) + 3V_S(q) + q^2 V_T(q) + 3W_{comb}(q)]$$

$$F_d(\rho) = \frac{1}{4} V_C''(0)$$

$$F_{so}(\rho) = \frac{1}{2} V_{SO}(0) + \int_0^1 dx\, x^3[V_{SO}(2xk_f) + 3W_{SO}(2xk_f)]$$

$$F_J(\rho) = \frac{3}{8k_f^2}\int_0^1 dx\left\{(2x^3 - x)[V_C(q) - V_S(q)] - x^3 q^2 V_T(q) + 3W_{comb}(q)\right\}$$

- Short-range pieces:

$$\bar{E}(\rho) = \frac{3\rho}{8}(C_S - C_T) + \frac{3\rho k_f^2}{20}(C_2 - C_1 - 3C_3 - C_6) + \frac{9\rho k_f^4}{140}(D_2 - 4D_1 + \dots)$$

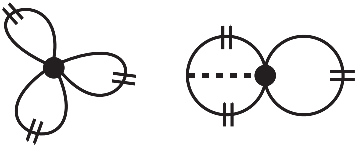
$$F_\tau(\rho) = \frac{\rho}{4}(C_2 - C_1 - 3C_3 - C_6) + \frac{\rho k_f^2}{4}(D_2 - 4D_1 - 12D_5 - 4D_{11})$$

$$F_d(\rho) = \frac{1}{32}(16C_1 - C_2 - 3C_4 - C_7) + \frac{k_f^2}{48}(9D_3 + 6D_4 - 9D_7 - 6D_8 + \dots)$$

$$F_{so}(\rho) = \frac{3}{8} C_5 + \frac{k_f^2}{6}(2D_9 + D_{10})$$

Three-body contributions at 1st order

- Leading order chiral 3N-interaction: contact + 1π-exchange + 2π-exch.
- LECs $c_E = -0.625, c_D = 2.06$ fitted to binding energies of ^{3}H and ^{4}He
- 3-body correlations in inhomogeneous nuclear many-body systems: factorized density-matrices in p-space $\Gamma(\vec{p}_1, \vec{q}_1)\,\Gamma(\vec{p}_2, \vec{q}_2)\,\Gamma(\vec{p}_3, -\vec{q}_1 - \vec{q}_2)$
- c_E- and c_D-terms:



$$\bar{E}(\rho) = -\frac{c_E k_f^6}{12\pi^4 f_\pi^4 \Lambda_\chi}$$

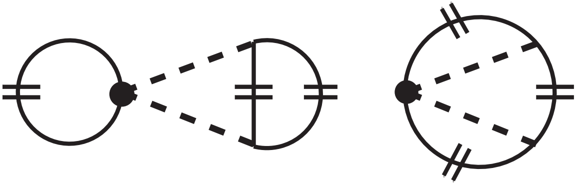
$$\bar{E}(\rho) = \frac{g_A c_D m_\pi^6}{(2\pi f_\pi)^4 \Lambda_\chi}\left\{\frac{u^6}{3} - \frac{3u^4}{4} + \frac{u^2}{8} + u^3 \arctan 2u - \frac{1+12u^2}{32}\ln(1+4u^2)\right\}$$

$$F_\tau(\rho) = \frac{2 g_A c_D m_\pi^4}{(4\pi f_\pi)^4 \Lambda_\chi}\left\{(1+2u^2)\ln(1+4u^2) - 4u^2\right\}$$

$$F_d(\rho) = \frac{g_A c_D m_\pi}{(4 f_\pi)^4 \pi^2 \Lambda_\chi}\left\{\frac{1}{2u}\ln(1+4u^2) - \frac{2u}{1+4u^2}\right\}$$

$$F_J(\rho) = \frac{3 g_A c_D m_\pi}{(4 f_\pi)^4 \pi^2 \Lambda_\chi}\left\{2u - \frac{1}{u} + \frac{1}{4u^3}\ln(1+4u^2)\right\}, \qquad u = \frac{k_f}{m_\pi}$$

Three-body contributions at 1st order



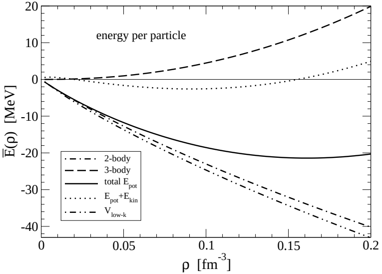
- 2π-exchange Hartree diagram prop. to $c_1 = -0.76$, $c_3 = -4.78$ (GeV^{-1})

$$\bar{E}(\rho) = \frac{g_A^2 m_\pi^6}{(2\pi f_\pi)^4}\Big\{(12c_1 - 10c_3)u^3 \arctan 2u - \frac{4}{3}c_3 u^6 + 6(c_3 - c_1)u^4 + (3c_1 - 2c_3)u^2 + \Big[\frac{1}{4}(2c_3 - 3c_1) + \frac{3u^2}{2}(3c_3 - 4c_1)\Big]\ln(1+4u^2)\Big\}$$

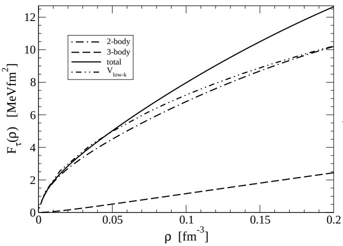
$$F_{so}(\rho) = \frac{3g_A^2 m_\pi}{(8\pi)^2 f_\pi^4}\Big\{\frac{2}{u}(4c_1 - 3c_3) - 4c_3 u + \Big[\frac{4}{u}(c_3 - c_1) + \frac{3c_3 - 4c_1}{2u^3}\Big]\ln(1+4u^2)\Big\}, \qquad u = \frac{k_f}{m_\pi}$$

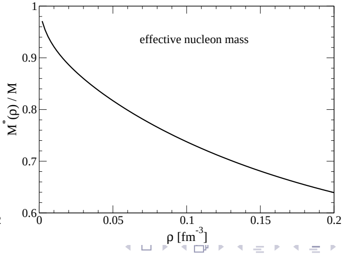
- 3-body spin-orbit coupling originally suggested by Fujita and Miyazawa
- More tedious to evaluate: 2π-exchange Fock diagram, $c_4 = 3.96$ GeV^{-1}

- Energy per particle: for 2-body part $V_{\mathrm{low-k}} \simeq V_{\mathrm{N^3LOW}}$



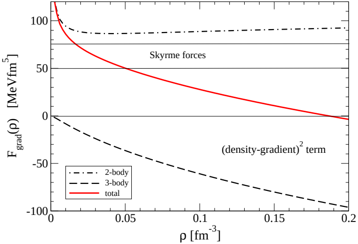
- Improved description: treat 2-body interaction to second order etc.
- Effective nucleon mass $M^*(\rho_0)$: in phenomenological reasonable range



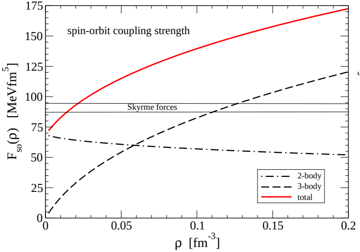


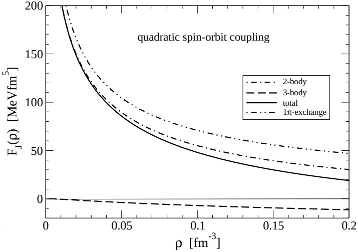
Results for isospin-symmetric nuclear systems

- Strength of surface term $(\vec{\nabla}\rho)^2$: fair agreement with phen. Skyrme forces



- Spin-orbit coupling strength





- 2-body contrib. mainly of short-range origin, sizeable 3-body spin-orbit c_3
- Expect reduction by second order π-exchange tensor interaction

Isovector part of nuclear energy density functional

- Isovector terms pertaining to different proton and neutron densities: relevant for long chains of stable isotopes and nuclei far from stability
- Up to second order in proton-neutron differences and spatial gradients

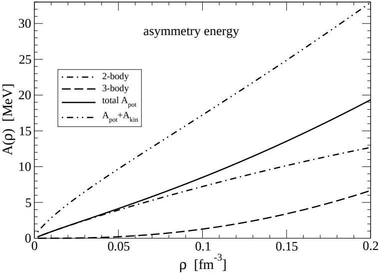
$$\mathcal{E}_{\rm iv}[\rho_p,\rho_n,\tau_p,\tau_n,\vec{J}_p,\vec{J}_n] = \frac{1}{\rho}(\rho_p-\rho_n)^2\,\tilde{A}(\rho) + \frac{1}{\rho}(\tau_p-\tau_n)(\rho_p-\rho_n)\,G_\tau(\rho)$$
$$+(\vec\nabla\rho_p-\vec\nabla\rho_n)^2\,G_\nabla(\rho) + (\vec\nabla\rho_p-\vec\nabla\rho_n)\cdot(\vec{J}_p-\vec{J}_n)\,G_{so}(\rho) + (\vec{J}_p-\vec{J}_n)^2\,G_J(\rho)$$

- $\tilde{A}(\rho)$ interacting part of nuclear matter asymmetry energy
- $G_\tau(\rho)$ splits effective proton and neutron masses prop. to local $\rho_p-\rho_n$
- $G_\nabla(\rho)$ isovector surface term, $G_{so}(\rho)$ isovector spin-orbit coupl. strength
- Adapt density-matrix expansion to asym. situation: $\to$ Fourier-transform

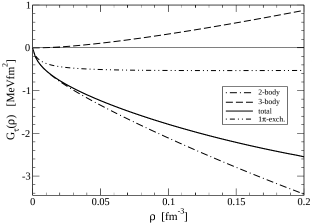
$$\Gamma_{\rm iv}(\vec p,\vec q\,) = \int d^3r\, e^{-i\vec q\cdot\vec r}\bigg\{\frac{\mathbf{1}+\boldsymbol{\tau}_3}{2}\,\theta(k_p-|\vec p\,|) + \frac{\mathbf{1}-\boldsymbol{\tau}_3}{2}\,\theta(k_n-|\vec p\,|)$$
$$+\frac{\pi^2}{4k_f^4}\Big[k_f\,\delta'(k_f-|\vec p\,|)-2\delta(k_f-|\vec p\,|)\Big]\bigg[\tau_p-\tau_n-\bigg(k_f^2+\frac{\vec\nabla^2}{4}\bigg)$$
$$\times(\rho_p-\rho_n)\bigg]\boldsymbol{\tau}_3 - \frac{3\pi^2}{4k_f^4}\,\delta(k_f-|\vec p\,|)\,(\vec\sigma\times\vec p\,)\cdot(\vec J_p-\vec J_n)\boldsymbol{\tau}_3\bigg\}$$

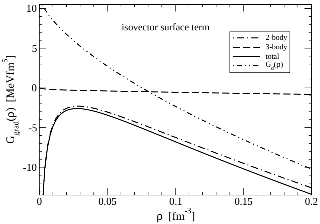
Fermi momenta: $\rho_p = k_p^3/3\pi^2,\ \ \rho_n = k_n^3/3\pi^2,\ \ \rho=\rho_p+\rho_n = 2k_f^3/3\pi^2$

- Asymmetry energy: $A(\rho_0) = 26.5\,\text{MeV}$, empirical value $(34 \pm 2)\text{MeV}$



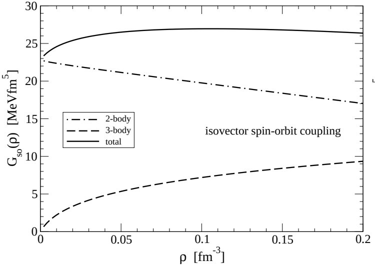
- Hartree-Fock approx. seems to work better for isovector quantities

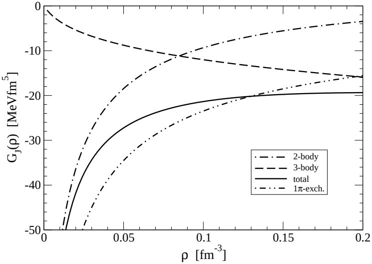




- $|G_\tau(\rho)| << F_\tau(\rho)$, from modern Sly forces $G_\nabla = -(11 \pm 5)\,\text{MeVfm}^5$

- Isovector spin-orbit coupling strength





- Small 3-body contrib., result close to Skyrme $G_{so} = \frac{1}{3} F_{so} \simeq 30\,\mathrm{MeVfm}^5$
- Isovector spin-orbit coupling in nuclei presently not well determined
- $G_J(\rho)$ and $F_J(\rho)$ are dominated by 1π-exchange, strong ρ-dependence

Challenges:

- Consistent calc. of EDF to 2nd order in many-body pertubation theory
- Energy denominators of intermediate states $\rightarrow$ further non-localities
- Generalized density-matrix expansion to 2nd order not yet formulated