

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

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 of choice for systematic calculation of medium-mass and heavy nuclei
- Non-relativistic (parametrized) Skyrme functionals and relativistic mean-field models ($\sigma + \omega$ -mesons) are widely and successfully used
- RMF: strong Lorentz scalar and vector mean-fields of opposite sign act coherently to generate nuclear spin-orbit interaction
- 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
- This work: Improved chiral NN-potential N^3LO + chiral 3N-interaction

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

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

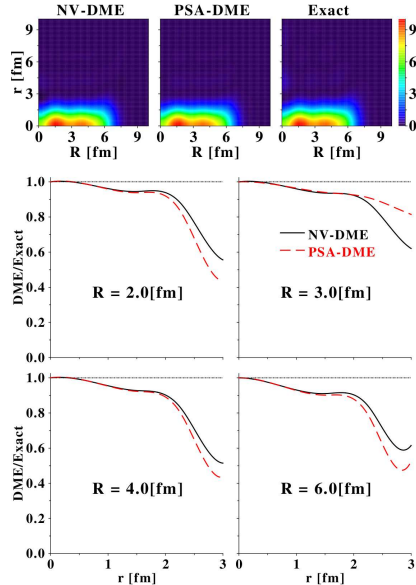
$\rho = 2k_f^3/3\pi^2$ local nucleon density, $\vec{J} = \sum_{\alpha} \Psi_{\alpha}^{\dagger} i \vec{\sigma} \times \vec{\nabla} \Psi_{\alpha}$ spin-orbit density

- 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

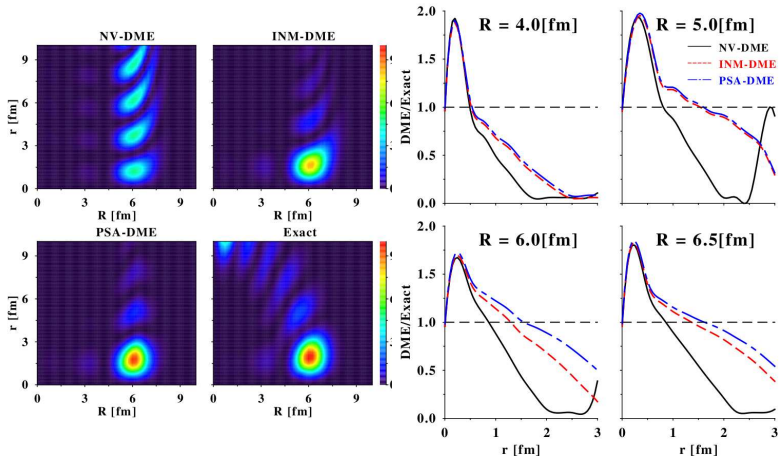
$$\Gamma(\vec{p}, \vec{q}) = \int d^3r e^{-i\vec{q} \cdot \vec{r}} \left\{ \theta(k_f - |\vec{p}|) + \frac{\pi^2}{4k_f^4} \left[k_f \delta'(k_f - |\vec{p}|) - 2\delta(k_f - |\vec{p}|) \right] \right. \\ \left. \times \left(\tau - \frac{3}{5} \rho k_f^2 - \frac{1}{4} \vec{\nabla}^2 \rho \right) - \frac{3\pi^2}{4k_f^4}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

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

- Comparison of density-matrix expansions: central interaction



- Comparison of density-matrix expansions: tensor interaction



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

- 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:

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

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

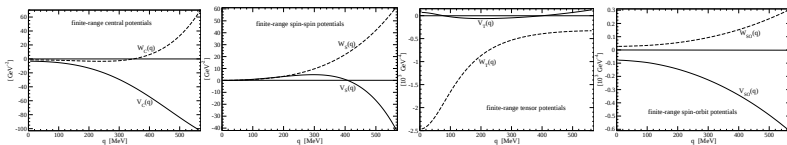
$$F_\nabla(\rho) = \frac{1}{4} \frac{\partial F_\tau(\rho)}{\partial \rho} + F_d(\rho)$$

- 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

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

$$V_{NN}^{(\pi)} = V_C(q) + \vec{\tau}_1 \cdot \vec{\tau}_2 W_C(q) + [V_S(q) + \vec{\tau}_1 \cdot \vec{\tau}_2 W_S(q)] \vec{\sigma}_1 \cdot \vec{\sigma}_2 \\ + [V_T(q) + \vec{\tau}_1 \cdot \vec{\tau}_2 W_T(q)] \vec{\sigma}_1 \cdot \vec{q} \vec{\sigma}_2 \cdot \vec{q} \\ + [V_{SO}(q) + \vec{\tau}_1 \cdot \vec{\tau}_2 W_{SO}(q)] i(\vec{\sigma}_1 + \vec{\sigma}_2) \cdot (\vec{q} \times \vec{p}),$$

- 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)

- 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:

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

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

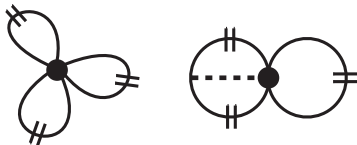
$$F_d(\rho) = \frac{1}{32} (16C_1 - C_2 - 3C_4 - C_7) + \frac{k_f^2}{48} (9D_3 + 6D_4 - 9D_7 - 6D_8 + \dots)$$

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



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 ^3H and ^4He
- 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:

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

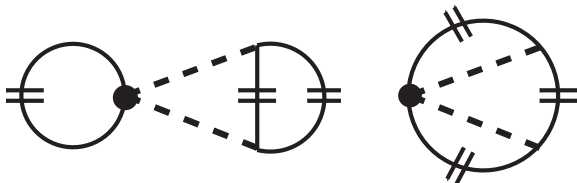
$$\bar{E}(\rho) = \frac{g_A c_D m_\pi^6}{(2\pi f_\pi)^4 \Lambda_\chi} \left\{ \frac{u^6}{3} - \frac{3u^4}{4} + \frac{u^2}{8} + u^3 \arctan 2u - \frac{1 + 12u^2}{32} \ln(1 + 4u^2) \right\}$$

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

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

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





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

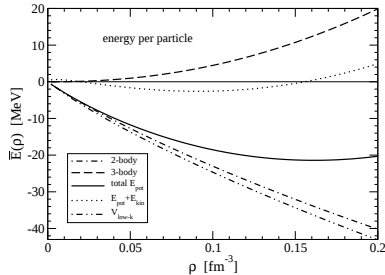
$$\bar{E}(\rho) = \frac{g_A^2 m_\pi^6}{(2\pi f_\pi)^4} \left\{ (12c_1 - 10c_3)u^3 \arctan 2u - \frac{4}{3}c_3 u^6 + 6(c_3 - c_1)u^4 \right. \\ \left. + (3c_1 - 2c_3)u^2 + \left[\frac{1}{4}(2c_3 - 3c_1) + \frac{3u^2}{2}(3c_3 - 4c_1) \right] \ln(1 + 4u^2) \right\}$$

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

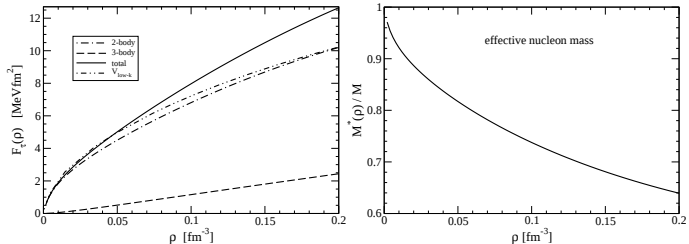
- 3-body spin-orbit coupling originally suggested by Fujita and Miyazawa
- Most tedious to evaluate: 2π -exchange Fock diagram, $c_4 = 3.96 \text{ GeV}^{-1}$

Results for isospin-symmetric nuclear systems

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

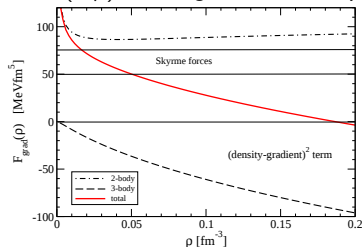


- Improved description: treat 2-body interaction to second order etc.
- Effective nucleon mass $M^*(\rho_0)$: in phenomenological reasonable range

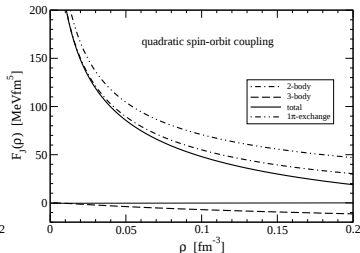
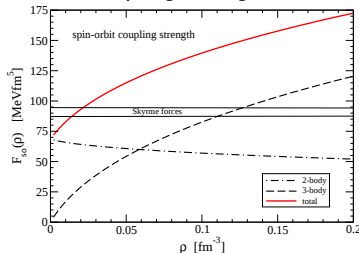


Results for isospin-symmetric nuclear systems

- 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



Isvector 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

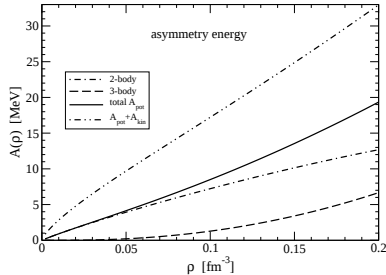
$$\begin{aligned}\mathcal{E}_{\text{iv}}[\rho_p, \rho_n, \tau_p, \tau_n, \vec{J}_p, \vec{J}_n] = & \frac{1}{\rho}(\rho_p - \rho_n)^2 \tilde{A}(\rho) + \frac{1}{\rho}(\tau_p - \tau_n)(\rho_p - \rho_n) G_\tau(\rho) \\ & + (\vec{\nabla}\rho_p - \vec{\nabla}\rho_n)^2 G_\nabla(\rho) + (\vec{\nabla}\rho_p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

- $\tilde{A}(\rho)$ 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: $\rightarrow$ Fourier-transform

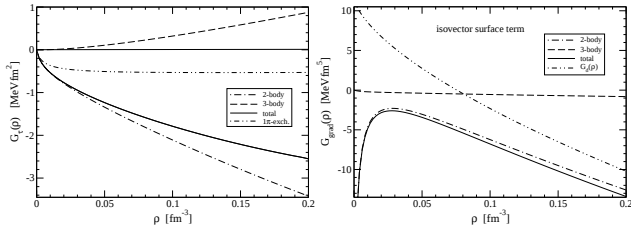
$$\begin{aligned}\Gamma_{\text{iv}}(\vec{p}, \vec{q}) = & \int d^3r e^{-i\vec{q}\cdot\vec{r}} \left\{ \frac{1+\tau_3}{2} \theta(k_p - |\vec{p}|) + \frac{1-\tau_3}{2} \theta(k_n - |\vec{p}|) \right. \\ & + \frac{\pi^2}{4k_f^4} \left[k_f \delta'(k_f - |\vec{p}|) - 2\delta(k_f - |\vec{p}|) \right] \left[\tau_p - \tau_n - \left(k_f^2 + \frac{\vec{\nabla}^2}{4} \right) \right. \\ & \left. \left. \times (\rho_p - \rho_n) \right] \tau_3 - \frac{3\pi^2}{4k_f^4} \delta(k_f - |\vec{p}|) (\vec{\sigma} \times \vec{p}) \cdot (\vec{J}_p - \vec{J}_n) \tau_3 \right\}\end{aligned}$$

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: $A(\rho_0) = 26.5$ MeV, empirical value (34 ± 2) MeV

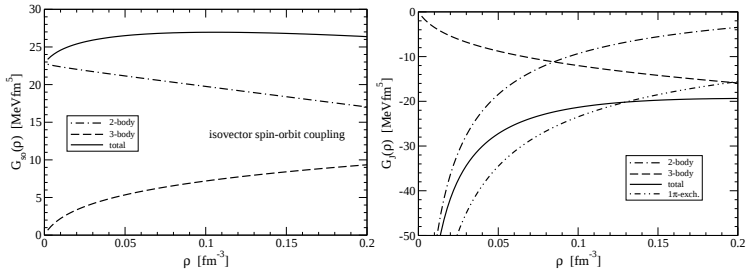


- Hartree-Fock approx. seems to work better for isovector quantities



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

- Isvector spin-orbit coupling strength



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

Challenge:

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