Skyrme functionals up to four gradients

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"Nuclear energy density functional method: going beyond the minefield"

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Disclaimer

This talk is not what I had in mind when accepting the invitation to present results on Skyrme N2LO at the workshop. Instead, Hofstadter's law applies:

It always takes longer than you expect, even when you take into account Hofstadter's Law.

Douglas Hofstadter, *Gödel, Escher, Bach: An Eternal Golden Braid* (1979)

- Bell & Skyrme's paper on a contact spin-orbit force

$$i(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2) \cdot (\mathbf{k}' \times \mathbf{k})[a-\tfrac{1}{2}(b\mathbf{k}^2+b^*\mathbf{k}'^2)+c\mathbf{k} \cdot \mathbf{k}']. \quad . \quad (16)$$

Bell & Skyrme, Philosophical Magazine 1 (1956) 1055

- Skyrme

7. D-Wave Interactions

The shortcomings of the assumed form (6) for the effective two-body interaction may be divided into incorrect *energy* dependence (i.e. upon $\mathbf{k}^2$ and $\mathbf{k}'^2$) and *angular* dependence (i.e. upon $\mathbf{k} \cdot \mathbf{k}'$). Since the range of momenta is much the same in all nuclei it is possible that the former type of error may not seriously affect matrix elements; on the other hand the small angular momenta involved in light nuclei mean that scattering at angles far from 0 or π may be important. The form of (6) corresponds to scattering only in S or P states; the analysis of nucleon-nucleon scattering at similar relative momenta indicates considerable amounts of D-wave (see section 9); it is expected therefore that an important correction to (6) might be represented by a term

$$t_{\mathrm{D}}[\mathbf{k}^2\mathbf{k}'^2-(\mathbf{k} \cdot \mathbf{k}')^2]. \qquad (7)$$

Skyrme, Nucl. Phys. 9 (1959) 615

- Brink & Boeker

general feature of all s-state interactions? We will show that there exist s-state interactions which give a reasonable fit to the binding energies of light nuclei and of nuclear matter. An example of such an interaction is

$$V(r) = A\delta(r)-B(\nabla^2\delta(r)+\delta(r)\nabla^2)+D\nabla^2\delta(r)\nabla^2. \qquad (33)$$

The matrix element in momentum space is

$$\langle k|V|k'\rangle = A+B(k^2+k'^2)+Dk^2k'^2. \qquad (34)$$

Brink and Boeker, Nucl. Phys. 91 (1967) 1

Jyväskylä:

- Carlsson, Dobaczewski, Kortelainen PRC 78 (2008) 044326: most general EDF with up to 6 gradients
- Raimondi, Carlsson, Dobaczewski, PRC 83, 054311 (2011): N3LO EDF from generator

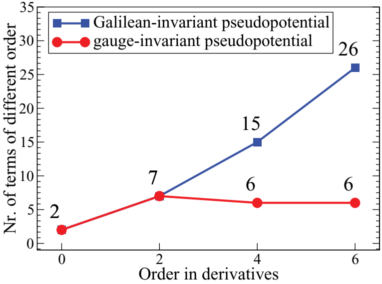

FIG. 1. (Color online) Number of terms of the pseudopotential (2), plotted as a function of the order in derivatives.

- Both mainly use a spherical representation of the gradient operators and densities ; cartesian expressions are also given, but leading to a non-standard representation already at NLO.
- Local gauge invariance is linked to the form of the continuity equation (Raimondi, Carlsson, Dobaczewski, Toivanen, PRC 84 (2011) 064303)
- public spherical code (Carlsson, Dobaczewski, Toivanen, Veselý, CPC 181 (2010) 1641)

Lyon group gets interested:

- Unpublished study of Skyrme's *D* wave that does not contribute to infinite matter
  Bennaceur, Pastore, Bender, Davesne, Duguet, Meyer, unpublished (2012)
- Study of the 6 locally gauge-invariant N2LO terms that do contribute to infinite matter

D. Davesne, A. Pastore, and J. Navarro, Skyrme effective pseudopotential up to the next-to-next-to-leading order, J. Phys. G 40, 095104 (2013).

D. Davesne, A. Pastore, and J. Navarro, Fitting N3LO pseudopotentials through central plus tensor Landau parameters, J. Phys. G 41, 065104 (2014).

D. Davesne, J. Navarro, P. Becker, R. Jodon, J. Meyer, and A. Pastore, Extended Skyrme pseudopotential deduced from infinite nuclear matter properties, Phys. Rev. C 91, 064303 (2015).

D. Davesne, J. Meyer, A. Pastore, and J. Navarro, Partial wave decomposition of the N3LO equation of state, Phys. Scr. 90, 114002 (2015).

D. Davesne, P. Becker, A. Pastore, and J. Navarro, Infinite matter properties and zero-range limit of non-relativistic finite range interactions, Ann. Phys. (NY) 375, 288 (2016).

D. Davesne, A. Pastore, and J. Navarro, Extended Skyrme equation of state in asymmetric nuclear matter, A & A 585 (2016) A83.

P. Becker, D. Davesne, J. Meyer, J. Navarro, and A. Pastore, Tools for incorporating a D-wave contribution in Skyrme energy density functionals, J. Phys. G 42, 034001 (2015).

- Parametrization for finite nuclei adding the 4 local central terms to a standard NLO form

  P. Becker, D. Davesne, J. Meyer, J. Navarro, and A. Pastore, Solution of Hartree-Fock-Bogoliubov equations and fitting procedure using the N2LO Skyrme pseudopotential in spherical symmetry, Phys. Rev. C 96, 044330 (2017).

  P. Becker, A. Pastore, D. Davesne, and J. Navarro, Error analysis of the parameters of the Skyrme N2LO pseudo-potential, Nuovo Cimento C 42, 88 (2019).

$$
\begin{aligned}
\mathcal{E}_t^{(4)}(\mathbf{r}) = \; & C_t^{(4)\Delta\rho} \big[\Delta\rho_t(\mathbf{r})\big]^2 + C_t^{(4)\Delta s} \big[\Delta\mathbf{s}_t(\mathbf{r})\big]^2 \\
& + C_t^{(4)M\rho} \Big\{ \rho_t(\mathbf{r})\, Q_t(\mathbf{r}) + \tau_t^2(\mathbf{r}) + 2 \sum_{\mu\nu} \tau_{t,\mu\nu}(\mathbf{r})\, \tau_{t,\mu\nu}(\mathbf{r}) - 2 \sum_{\mu\nu} \tau_{t,\mu\nu}(\mathbf{r}) \big[\nabla_\mu \nabla_\nu \rho_t(\mathbf{r})\big] \\
& \qquad - \big[\boldsymbol{\nabla}\cdot\mathbf{j}_t(\mathbf{r})\big]^2 - 4\, \mathbf{j}_t(\mathbf{r})\cdot\boldsymbol{\Pi}_t(\mathbf{r}) \Big\} \\
& + C_t^{(4)Ms} \Big\{ \mathbf{s}_t(\mathbf{r})\cdot\mathbf{S}_t(\mathbf{r}) + \mathbf{T}_t^2(\mathbf{r}) + 2 \sum_{\mu\nu\kappa} K_{t,\mu\nu\kappa}(\mathbf{r})\, K_{t,\mu\nu\kappa}(\mathbf{r}) - 2 \sum_{\mu\nu\kappa} K_{t,\mu\nu\kappa}(\mathbf{r}) \big[\nabla_\mu \nabla_\nu s_{t,\kappa}(\mathbf{r})\big] \\
& \qquad - \sum_\nu \Big[\sum_\mu \nabla_\mu J_{t,\mu\nu}(\mathbf{r})\Big] \Big[\sum_\kappa \nabla_\kappa J_{t,\kappa\nu}(\mathbf{r})\Big] - 4 \sum_{\mu\nu} J_{t,\mu\nu}(\mathbf{r})\, V_{t,\mu\nu}(\mathbf{r}) \Big\}
\end{aligned}
$$

4 additional real densities

$Q_q(\mathbf{r}) \equiv \Delta\,\Delta'\, \rho_q(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}$,	$V_{q,\mu\nu}(\mathbf{r}) \equiv -\frac{i}{2}\,(\nabla_\mu - \nabla'_\mu)\,(\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}')\, s_{q,\nu}(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}$	time even
$\mathbf{S}_q(\mathbf{r}) \equiv \Delta\,\Delta'\, \mathbf{s}_q(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}$,	$\Pi_{q,\mu}(\mathbf{r}) \equiv -\frac{i}{2}\,(\nabla_\mu - \nabla'_\mu)\,(\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}')\, \rho_q(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}$,	time odd

and 2 in general complex densities

$\tau_{q,\mu\nu}(\mathbf{r}) \equiv \nabla_\mu\, \nabla'_\nu\, \rho_q(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}$,	$K_{q,\mu\nu\kappa}(\mathbf{r}) \equiv \nabla_\mu\, \nabla'_\nu\, s_{q,\kappa}(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}$,	neither

Ryssens and Bender, PRC 104 (2021) 044308

Problems with the extension of the standard Skyrme notation to N2LO and beyond

- How to define densities that are real and either time-even or time-odd?
- densities might be redundant

$$\Im\{\tau_{q,\mu\nu}(\mathbf{r})\} = \tfrac{1}{2}\left[\nabla_\mu \, j_{q,\nu}(\mathbf{r}) - \nabla_\nu \, j_{q,\mu}(\mathbf{r})\right].$$

- How to ensure to work with linearly independent densities?

  Alternative second-order kinetic density

$$\mathcal{T}_q(\mathbf{r}) \equiv (\boldsymbol{\nabla}' \cdot \boldsymbol{\nabla})\,(\boldsymbol{\nabla}' \cdot \boldsymbol{\nabla}) \;\; \rho_q(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'} \; .$$

  that is linearly dependent on $Q_q(\mathbf{r})$

$$\mathcal{T}_q(\mathbf{r}) = Q_q(\mathbf{r}) + \Delta\tau_q(\mathbf{r}) - \sum_{\mu\nu} \nabla_\mu \nabla_\nu \tau_{q,\mu\nu}(\mathbf{r})\,.$$

- Mnemonic problems with notation for additional densities and corresponding potentials

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New symbolic-computation friendly notation for generic densities and currents

$$D_q^{A,B}(\mathbf{r}) \equiv \Re\{\hat{A}'\hat{B}\,\rho_q(\mathbf{r},\mathbf{r}')\}\Big|_{\mathbf{r}=\mathbf{r}'} = +\tfrac{1}{2}\,(\hat{A}'\hat{B} + \hat{A}\hat{B}')\,\rho_q(\mathbf{r},\mathbf{r}')\Big|_{\mathbf{r}=\mathbf{r}'}$$

$$C_q^{A,B}(\mathbf{r}) \equiv \Im\{\hat{A}'\hat{B}\,\rho_q(\mathbf{r},\mathbf{r}')\}\Big|_{\mathbf{r}=\mathbf{r}'} = -\tfrac{\mathrm{i}}{2}\,(\hat{A}'\hat{B} - \hat{A}\hat{B}')\,\rho_q(\mathbf{r},\mathbf{r}')\Big|_{\mathbf{r}=\mathbf{r}'}$$

$$D_q^{A,B\sigma}(\mathbf{r}) \equiv \Re\{\hat{A}'\hat{B}\,\mathbf{s}_q(\mathbf{r},\mathbf{r}')\}\Big|_{\mathbf{r}=\mathbf{r}'} = +\tfrac{1}{2}\,(\hat{A}'\hat{B} + \hat{A}\hat{B}')\,\mathbf{s}_q(\mathbf{r},\mathbf{r}')\Big|_{\mathbf{r}=\mathbf{r}'}$$

$$C_q^{A,B\sigma}(\mathbf{r}) \equiv \Im\{\hat{A}'\hat{B}\,\mathbf{s}_q(\mathbf{r},\mathbf{r}')\}\Big|_{\mathbf{r}=\mathbf{r}'} = -\tfrac{\mathrm{i}}{2}\,(\hat{A}'\hat{B} - \hat{A}\hat{B}')\,\mathbf{s}_q(\mathbf{r},\mathbf{r}')\Big|_{\mathbf{r}=\mathbf{r}'}$$

Cartesian tensor indices of the gradients and spin densities are suppressed for sake of compact notation.

Advantages of the notation

- **Extensibility**: the notation can be extended indefinitely, up to any order in derivatives.
- **Clarity**: the operator structure of any given density is incorporated directly into the notation.
- **Reality**: By construction, all normal $D(\mathbf{r})$ and $C(\mathbf{r})$ objects are real spatial functions when doing single-reference EDF calculations.
- **Time-reversal**: $D(\mathbf{r})$ and $C(\mathbf{r})$ objects have definite behavior under time-reversal: they are either time-even or time-odd, never mixed.

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New notation and definitions

Time-reversal

$$\left[D_q^{A,B}\right]^T(\mathbf{r}) = +D_q^{A,B}(\mathbf{r}),$$

$$\left[C_q^{A,B}\right]^T(\mathbf{r}) = -C_q^{A,B}(\mathbf{r}),$$

$$\left[D_q^{A,B\sigma}\right]^T(\mathbf{r}) = -D_q^{A,B\sigma}(\mathbf{r}),$$

$$\left[C_q^{A,B\sigma}\right]^T(\mathbf{r}) = +C_q^{A,B\sigma}(\mathbf{r}).$$

Symmetries:

$$D_q^{A,B}(\mathbf{r}) = +D_q^{B,A}(\mathbf{r})$$

$$C_q^{A,B}(\mathbf{r}) = -C_q^{B,A}(\mathbf{r})$$

$$D_q^{A,B\sigma}(\mathbf{r}) = +D_q^{B,A\sigma}(\mathbf{r})$$

$$C_q^{A,B\sigma}(\mathbf{r}) = -C_q^{B,A\sigma}(\mathbf{r})$$

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Recoupling of gradients:

$$D_q^{\nabla A,B}(\mathbf{r}) = \nabla D_q^{A,B}(\mathbf{r}) - D_q^{A,\nabla B}(\mathbf{r})\,, \qquad C_q^{\nabla A,B}(\mathbf{r}) = \nabla C_q^{A,B}(\mathbf{r}) - C_q^{A,\nabla B}(\mathbf{r})\,.$$

If a is non-zero:

$$D^{\nabla^a,\nabla^b}_{q,\mu_1\mu_2\ldots\mu_{a+b}}(\mathbf{r}) = (-1)^a D^{1,\nabla^{a+b}}_{q,\mu_1\mu_2\ldots\mu_{a+b}}(\mathbf{r}) + \sum_{n=1}^{a}(-1)^{n+1}\left(\prod_{k=1}^{n}\nabla_{\mu_k}\right) D^{\nabla^{a-n},\nabla^b}_{q,\mu_{n+1}\ldots\mu_{a+b}}(\mathbf{r})$$

If b is non-zero:

$$D^{\nabla^a,\nabla^b}_{q,\mu_1\mu_2\ldots\mu_{a+b}}(\mathbf{r}) = (-1)^b D^{\nabla^{a+b},1}_{q,\mu_1\mu_2\ldots\mu_{a+b}}(\mathbf{r}) + \sum_{n=1}^{b}(-1)^{n+1}\left(\prod_{k=0}^{n-1}\nabla_{\mu_{a+b-k}}\right) D^{\nabla^a,\nabla^{b-n}}_{q,\mu_1\mu_2\ldots\mu_{a+b-n}}(\mathbf{r})\,.$$

If both a and b are non-zero:

$$2D^{\nabla^a,\nabla^b}_{q,\mu_1\mu_2\ldots\mu_{a+b}}(\mathbf{r}) = \left[(-1)^a + (-1)^b\right] D^{1,\nabla^{a+b}}_{q,\mu_1\mu_2\ldots\mu_{a+b}}(\mathbf{r}) + \cdots$$

From these relations follows that

If $a+b$ is **odd**, then $\left\{ \begin{array}{c} D_q^{\nabla^a,\nabla^b}(\mathbf{r}) \\ D_q^{\nabla^a,\nabla^b\sigma}(\mathbf{r}) \end{array} \right\}$ is reducible.

If $a+b$ is **even**, then $\left\{ \begin{array}{c} C_q^{\nabla^a,\nabla^b}(\mathbf{r}) \\ C_q^{\nabla^a,\nabla^b\sigma}(\mathbf{r}) \end{array} \right\}$ is reducible.

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NLO:

$$\rho_q(\mathbf{r}) \to D_q^{1,1}(\mathbf{r})$$
$$s_{q,\mu}(\mathbf{r}) \to D_{q,\mu}^{1,\sigma}(\mathbf{r})$$
$$\tau_q(\mathbf{r}) \to D_q^{(\nabla,\nabla)}(\mathbf{r})$$
$$T_{q,\mu}(\mathbf{r}) \to D_{q,\mu}^{(\nabla,\nabla)\sigma}(\mathbf{r})$$
$$F_{q,\mu}(\mathbf{r}) \to D_{q,\mu}^{\nabla,(\nabla\sigma)}(\mathbf{r})$$
$$j_{q,\mu}(\mathbf{r}) \to C_{q,\mu}^{1,\nabla}(\mathbf{r})$$
$$J_{q,\mu\nu}(\mathbf{r}) \to C_{q,\mu\nu}^{1,\nabla\sigma}(\mathbf{r})$$
$$\mathbf{J}_q\mathbf{r}) \to \mathbf{C}_q^{1,\nabla\times\sigma}(\mathbf{r})$$

N2LO as used before

$$Q_q(\mathbf{r}) \to D_q^{\Delta,\Delta}(\mathbf{r})\,,$$
$$S_{q,\mu}(\mathbf{r}) \to D_{q,\mu}^{\Delta,\Delta\sigma}(\mathbf{r})$$
$$\Pi_{q,\mu}(\mathbf{r}) \to C_{q,\mu}^{(\nabla,\nabla)\nabla}(\mathbf{r})$$
$$V_{q,\mu\nu}(\mathbf{r}) \to C_{q,\mu\nu}^{(\nabla,\nabla)\nabla\sigma}(\mathbf{r})$$
$$\tau_{q,\mu\nu}(\mathbf{r}) \to D_{q,\nu\mu}^{\nabla,\nabla}(\mathbf{r}) + \frac{\mathrm{i}}{2}\left[\nabla_\nu C_{q,\mu}^{1,\nabla}(\mathbf{r}) - \nabla_\mu C_{q,\nu}^{1,\nabla}(\mathbf{r})\right]$$
$$K_{q,\mu\nu\kappa}(\mathbf{r}) \to D_{q,\nu\mu\kappa}^{\nabla,\nabla\sigma}(\mathbf{r}) + \frac{\mathrm{i}}{2}\left[\nabla_\nu C_{q,\mu}^{1,\nabla\sigma}(\mathbf{r}) - \nabla_\mu C_{q,\nu}^{1,\nabla\sigma}(\mathbf{r})\right]$$

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$$\tilde{D}_q^{A,B}(\mathbf{r}) \equiv \sum_{j<k} \kappa_{kj} \big(\hat{A}'\hat{B} + \hat{A}\hat{B}'\big) \Re\{\tilde{\varrho}_{jk}(\mathbf{r},\mathbf{r}')\}\Big|_{\mathbf{r}=\mathbf{r}'} \, ,$$

$$\tilde{C}_q^{A,B}(\mathbf{r}) \equiv \sum_{j<k} \kappa_{kj} \big(\hat{A}'\hat{B} + \hat{A}\hat{B}'\big) \Im\{\tilde{\varrho}_{jk}(\mathbf{r},\mathbf{r}')\}\Big|_{\mathbf{r}=\mathbf{r}'} \, ,$$

$$\tilde{D}_{q,\mu}^{A,B\sigma}(\mathbf{r}) \equiv \sum_{j<k} \kappa_{kj} \big(\hat{A}'\hat{B} - \hat{A}\hat{B}'\big) \Re\{\tilde{\varsigma}_{jk,\mu}(\mathbf{r},\mathbf{r}')\}\Big|_{\mathbf{r}=\mathbf{r}'}$$

$$\tilde{C}_{q,\mu}^{A,B\sigma}(\mathbf{r}) \equiv \sum_{j<k} \kappa_{kj} \big(\hat{A}'\hat{B} - \hat{A}\hat{B}'\big) \Im\{\tilde{\varsigma}_{jk,\mu}(\mathbf{r},\mathbf{r}')\}\Big|_{\mathbf{r}=\mathbf{r}'}$$

The spatial objects are a $S = 0$, $T_3 = \pm 1$ two-body wave function

$$\tilde{\varrho}_{jk}(\mathbf{r},\mathbf{r}') \equiv \sum_{\sigma} \sigma \, \psi_j(\mathbf{r}',\sigma) \, \psi_k(\mathbf{r},-\sigma) \, ,$$

and the three components of a $S = 1$, $T_3 = \pm 1$ two-body wave function

$$\tilde{\varsigma}_{jk,\mu}(\mathbf{r},\mathbf{r}') \equiv \sum_{\sigma,\sigma'} \sigma' \, \psi_j(\mathbf{r}',\sigma') \, \psi_k(\mathbf{r},\sigma) \, \langle -\sigma' | \hat{\sigma}_\mu | \sigma \rangle$$

- The real and imaginary parts of $\tilde{\varrho}_{jk}(\mathbf{r},\mathbf{r}')$ and $\tilde{\varsigma}_{jk,\mu}(\mathbf{r},\mathbf{r}')$ have different spatial symmetries.
- κ cannot always be chosen to be real, such that all pair densities might be complex.
- The definition guarantees that when κ is complex, the pair densities and currents still adopt the symmetries of the single-particle states.

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Computational considerations

To reduce memory requirements and to reduce the computational cost of constructing densities and applying the corresponding term in the single-particle Hamiltonian

- Couple gradients to Laplacians whenever possible: use

$$C^{\Delta,\nabla\sigma}_{q,\mu\nu}(\mathbf{r}) = \Im\Big\{ \sum_{jk} \rho_{kj} \sum_{\kappa} \big[\Delta \Psi^{\dagger}_{j}(\mathbf{r})\big] \big[\nabla_{\mu} \hat{\sigma}_{\nu} \Psi_{k}(\mathbf{r})\big] \Big\}$$

instead of

$$V_{q,\mu\nu}(\mathbf{r}) = C^{(\nabla,\nabla)\nabla\sigma}_{q,\mu\nu}(\mathbf{r}) = \Im\Big\{ \sum_{jk} \rho_{kj} \sum_{\kappa} \big[\nabla_{\kappa} \Psi^{\dagger}_{j}(\mathbf{r})\big] \big[\nabla_{\kappa}\nabla_{\mu} \hat{\sigma}_{\nu} \Psi_{k}(\mathbf{r})\big] \Big\}$$

$$= - C^{\Delta,\nabla\sigma}_{q,\mu\nu}(\mathbf{r}) + \tfrac{1}{2}\big[\Delta C^{1,\nabla\sigma}_{q,\mu\nu}(\mathbf{r})\big] - \tfrac{1}{2}\sum_{\kappa}\big[\nabla_{\kappa}\nabla_{\mu} C^{1,\nabla\sigma}_{q,\kappa\nu}(\mathbf{r})\big]$$

- Balance the number of derivative operators on the "left" (acting on $\mathbf{r}'$) and on the "right" (acting on $\mathbf{r}$)

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NLO:

$$\begin{aligned}
\rho_q(\mathbf{r}) &\to D_q^{1,1}(\mathbf{r}) \\
s_{q,\mu}(\mathbf{r}) &\to D_{q,\mu}^{1,\sigma}(\mathbf{r}) \\
\tau_q(\mathbf{r}) &\to D_q^{(\nabla,\nabla)}(\mathbf{r}) \\
T_{q,\mu}(\mathbf{r}) &\to D_{q,\mu}^{(\nabla,\nabla)\sigma}(\mathbf{r}) \\
F_{q,\mu}(\mathbf{r}) &\to D_{q,\mu}^{\nabla,(\nabla\sigma)}(\mathbf{r}) \\
j_{q,\mu}(\mathbf{r}) &\to C_{q,\mu}^{1,\nabla}(\mathbf{r}) \\
J_{q,\mu\nu}(\mathbf{r}) &\to C_{q,\mu\nu}^{1,\nabla\sigma}(\mathbf{r}) \\
\mathbf{J}_q\mathbf{r}) &\to \mathbf{C}_q^{1,\nabla\times\sigma}(\mathbf{r})
\end{aligned}$$

N2LO as used before

$$\begin{aligned}
Q_q(\mathbf{r}) &\to D_q^{\Delta,\Delta}(\mathbf{r})\,, \\
S_{q,\mu}(\mathbf{r}) &\to D_{q,\mu}^{\Delta,\Delta\sigma}(\mathbf{r}) \\
C_{q,\mu}^{\Delta,\nabla}&(\mathbf{r}) \\
C_{q,\mu\nu}^{\Delta,\nabla\sigma}&(\mathbf{r}) \\
D_{q,\nu\mu}^{\nabla,\nabla}&(\mathbf{r}) \\
D_{q,\nu\mu\kappa}^{\nabla,\nabla\sigma}&(\mathbf{r})
\end{aligned}$$

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$$\mathcal{E}^{(0)}_{\rm Sk,e}(\mathbf{r}) = \sum_{t=0,1} \Big[A^{(0,1)}_{t,\rm e} (D^{1,1}_t)^2 + A^{(0,2)}_{t,\rm e} (D^{1,1}_0)^\alpha (D^{1,1}_t)^2 \Big]$$

$$\mathcal{E}^{(0)}_{\rm Sk,o}(\mathbf{r}) = \sum_{t=0,1} \Big[A^{(0,1)}_{t,\rm o} \mathbf{D}^{1,\sigma}_t \cdot \mathbf{D}^{1,\sigma}_t + A^{(0,2)}_{t,\rm o} (D^{1,1}_0)^\alpha \, \mathbf{D}^{1,\sigma}_t \cdot \mathbf{D}^{1,\sigma}_t \Big]$$

$$\mathcal{E}^{(2)}_{\rm Sk,e}(\mathbf{r}) = \sum_{t=0,1} \Big[A^{(2,1)}_{t,\rm e} D^{1,1}_t (\Delta D^{1,1}_t) + A^{(2,2)}_{t,\rm e} D^{1,1}_t D^{(\nabla,\nabla)}_t + A^{(2,3)}_{t,\rm e} \sum_{\mu\nu} C^{1,\nabla\sigma}_{t,\mu\nu} C^{1,\nabla\sigma}_{t,\mu\nu} + A^{(2,4)}_{t,\rm e} D^{1,1}_t (\nabla \cdot \mathbf{C}^{1,\nabla\times\sigma}_t) \Big]$$

$$\mathcal{E}^{(2)}_{\rm Sk,o}(\mathbf{r}) = \sum_{t=0,1} \Big[A^{(2,1)}_{t,\rm o} \mathbf{D}^{1,\sigma}_t \cdot (\Delta \mathbf{D}^{1,\sigma}_t) + A^{(2,2)}_{t,\rm o} \mathbf{D}^{1,\sigma}_t \cdot \mathbf{D}^{(\nabla,\nabla)\sigma}_t + A^{(2,3)}_{t,\rm o} \mathbf{C}^{1,\nabla}_t \cdot \mathbf{C}^{1,\nabla}_t + A^{(2,4)}_{t,\rm o} \mathbf{D}^{1,\sigma}_t \cdot (\boldsymbol{\nabla} \times \mathbf{C}^{1,\nabla}_t) \Big]$$

$$\begin{aligned}\mathcal{E}^{(4)}_{\rm Sk,e}(\mathbf{r}) = \sum_{t=0,1} \Big[& A^{(4,1)}_{t,\rm e} (\Delta D^{1,1}_t)(\Delta D^{1,1}_t) + A^{(4,2)}_{t,\rm e} D^{1,1}_t \, D^{\Delta,\Delta}_t + A^{(4,3)}_{t,\rm e} D^{(\nabla,\nabla)}_t D^{(\nabla,\nabla)}_t \\ & + A^{(4,4)}_{t,\rm e} \sum_{\mu\nu} D^{\nabla,\nabla}_{t,\mu\nu} D^{\nabla,\nabla}_{t,\mu\nu} + A^{(4,5)}_{t,\rm e} \sum_{\mu\nu} D^{\nabla,\nabla}_{t,\mu\nu} (\nabla_\mu \nabla_\nu D^{1,1}_t) \\ & + A^{(4,6)}_{t,\rm e} \sum_{\mu\nu} C^{1,\nabla\sigma}_{t,\mu\nu} (\Delta C^{1,\nabla\sigma}_{t,\mu\nu}) + A^{(4,7)}_{t,\rm e} \sum_{\mu\nu\kappa} (\nabla_\mu C^{1,\nabla\sigma}_{t,\mu\kappa})(\nabla_\nu C^{1,\nabla\sigma}_{t,\nu\kappa}) + A^{(4,8)}_{t,\rm e} \sum_{\mu\nu} C^{1,\nabla\sigma}_{t,\mu\nu} C^{\Delta,\nabla\sigma}_{t,\mu\nu} \Big]\end{aligned}$$

$$\begin{aligned}\mathcal{E}^{(4)}_{\rm Sk,o}(\mathbf{r}) = \sum_{t=0,1} \Big[& A^{(4,1)}_{t,\rm o} (\Delta \mathbf{D}^{1,\sigma}_t) \cdot (\Delta \mathbf{D}^{1,\sigma}_t) + A^{(4,2)}_{t,\rm o} \mathbf{D}^{1,\sigma}_t \cdot \mathbf{D}^{\Delta,\Delta\sigma}_t + A^{(4,3)}_{t,\rm o} \mathbf{D}^{(\nabla,\nabla)\sigma}_t \cdot \mathbf{D}^{(\nabla,\nabla)\sigma}_t \\ & + A^{(4,4)}_{t,\rm o} \sum_{\mu\nu\kappa} D^{\nabla,\nabla\sigma}_{\mu\nu\kappa} D^{\nabla,\nabla\sigma}_{\mu\nu\kappa} + A^{(4,5)}_{t,\rm o} \sum_{\mu\nu\kappa} D^{\nabla,\nabla\sigma}_{\mu\nu\kappa} (\nabla_\mu \nabla_\nu D^{1,\sigma}_\kappa) \\ & + A^{(4,6)}_{t,\rm o} \mathbf{C}^{1,\nabla}_t \cdot (\Delta \mathbf{C}^{1,\nabla}_t) + A^{(4,7)}_{t,\rm o} (\boldsymbol{\nabla} \cdot \mathbf{C}^{1,\nabla}_t)(\boldsymbol{\nabla} \cdot \mathbf{C}^{1,\nabla}_t) + A^{(4,8)}_{t,\rm o} \mathbf{C}^{1,\nabla}_t \cdot \mathbf{C}^{\Delta,\nabla}_t \Big]\end{aligned}$$

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$$h_q(\mathbf{r}\sigma, \mathbf{r}'\sigma') = \sum_{n=0}^{4} \left[h^{(n)}_{q,\mathrm{e}}(\mathbf{r}\sigma, \mathbf{r}'\sigma') + h^{(n)}_{q,\mathrm{o}}(\mathbf{r}\sigma, \mathbf{r}'\sigma') \right]$$

$$h^{(0)}_{q,\mathrm{e}}(\mathbf{r}\sigma, \mathbf{r}'\sigma') = \delta_{\sigma\sigma'} \, F^{1,1}_q(\mathbf{r}) \, \delta_{\mathbf{r}\mathbf{r}'} \quad ,$$

$$h^{(0)}_{q,\mathrm{o}}(\mathbf{r}\sigma, \mathbf{r}'\sigma') = \sum_{\mu} \langle \sigma | \hat{\sigma}_\mu | \sigma' \rangle \, F^{1,\sigma}_{q,\mu}(\mathbf{r}) \, \delta_{\mathbf{r}\mathbf{r}'} \, ,$$

$$h^{(1)}_{q,\mathrm{e}}(\mathbf{r}\sigma, \mathbf{r}'\sigma') = -\tfrac{\mathrm{i}}{2} \sum_{\mu\nu} \langle \sigma | \hat{\sigma}_\nu | \sigma' \rangle \left[\nabla_\mu \, G^{1,\nabla\sigma}_{q,\mu\nu}(\mathbf{r}) + G^{1,\nabla\sigma}_{q,\mu\nu}(\mathbf{r}) \, \nabla_\mu \right] \delta_{\mathbf{r}\mathbf{r}'} \, ,$$

$$h^{(1)}_{q,\mathrm{o}}(\mathbf{r}\sigma, \mathbf{r}'\sigma') = -\tfrac{\mathrm{i}}{2} \, \delta_{\sigma\sigma'} \sum_{\mu} \left[\nabla_\mu \, G^{1,\nabla}_{q,\mu}(\mathbf{r}) + G^{1,\nabla}_{q,\mu}(\mathbf{r}) \, \nabla_\mu \right] \delta_{\mathbf{r}\mathbf{r}'} \, ,$$

$$h^{(2)}_{q,\mathrm{e}}(\mathbf{r}\sigma, \mathbf{r}'\sigma') = -\delta_{\sigma\sigma'} \sum_{\mu\nu} \nabla_\mu \, F^{\nabla,\nabla}_{q,\mu\nu}(\mathbf{r}) \, \nabla_\nu \, \delta_{\mathbf{r}'\mathbf{r}} \, ,$$

$$h^{(2)}_{q,\mathrm{o}}(\mathbf{r}\sigma, \mathbf{r}'\sigma') = -\sum_{\mu\nu\kappa} \langle \sigma | \hat{\sigma}_\kappa | \sigma' \rangle \nabla_\mu \, F^{\nabla,\nabla\sigma}_{q,\mu\nu\kappa}(\mathbf{r}) \, \nabla_\nu \, \delta_{\mathbf{r}\mathbf{r}'} \, ,$$

$$h^{(3)}_{q,\mathrm{e}}(\mathbf{r}\sigma, \mathbf{r}'\sigma') = -\tfrac{\mathrm{i}}{2} \sum_{\mu\nu} \langle \sigma | \hat{\sigma}_\nu | \sigma' \rangle \left[\nabla_\mu \, G^{\Delta,\nabla\sigma}_{q,\mu\nu}(\mathbf{r}) \, \Delta + \Delta \, G^{\Delta,\nabla\sigma}_{q,\mu\nu}(\mathbf{r}) \, \nabla_\mu \right] \delta_{\mathbf{r}\mathbf{r}'} \, ,$$

$$h^{(3)}_{q,\mathrm{o}}(\mathbf{r}\sigma, \mathbf{r}'\sigma') = -\tfrac{\mathrm{i}}{2} \, \delta_{\sigma\sigma'} \sum_{\mu} \left[\nabla_\mu \, G^{\Delta,\nabla}_{q,\mu}(\mathbf{r}) \, \Delta + \Delta \, G^{\Delta,\nabla}_{q,\mu}(\mathbf{r}) \, \nabla_\mu \right] \delta_{\mathbf{r}\mathbf{r}'} \, ,$$

$$h^{(4)}_{q,\mathrm{e}}(\mathbf{r}\sigma, \mathbf{r}'\sigma') = \delta_{\sigma\sigma'} \, \Delta \, F^{\Delta,\Delta}_q(\mathbf{r}) \, \Delta \, \delta_{\mathbf{r}\mathbf{r}'} \quad ,$$

$$h^{(4)}_{q,\mathrm{o}}(\mathbf{r}\sigma, \mathbf{r}'\sigma') = \sum_{\mu} \langle \sigma | \hat{\sigma}_\mu | \sigma' \rangle \Delta \, F^{\Delta,\Delta\sigma}_{q,\mu}(\mathbf{r}) \, \Delta \, \delta_{\mathbf{r}\mathbf{r}'} \, .$$

SN2LO1

TABLE VII. Infinite matter properties at saturation for SN2LO1 and SLy5 [24]. See text for details.

	SN2LO1	SLy5
ρ_0 (fm^{-3})	0.162	0.1603
E/A(ρ_0) (MeV)	−15.948	−15.98
K_∞ (MeV)	221.9	229.92
J (MeV)	31.95	32.03
L (MeV)	48.9	48.15
m^*/m	0.709	0.696

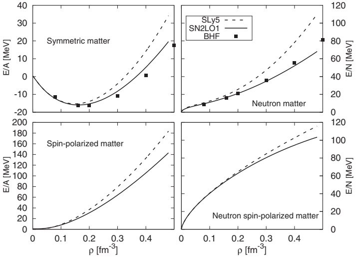


FIG. 9. Equation of state for SNM and PNM obtained with the N2LO Skyrme interaction. The squares represent the values obtained from BHF calculations.

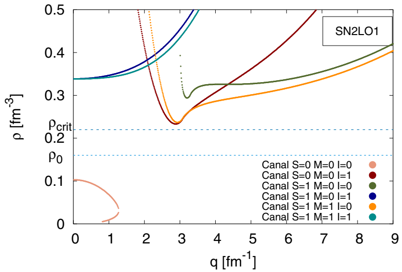
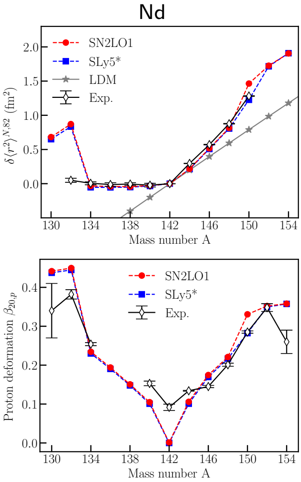
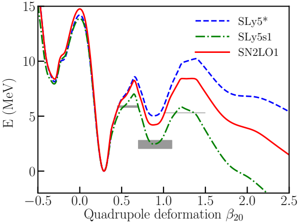
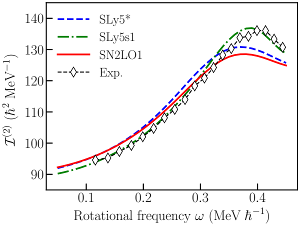


FIG. 8. Critical densities in SNM as a function of transferred momentum q. The horizontal dashed lines represent the saturation density ρ_0 and the critical density $\rho_{\rm crit}$.

Becker, Davesne, Meyer, Navarro, Pastore, PRC 96 (2017) 044330

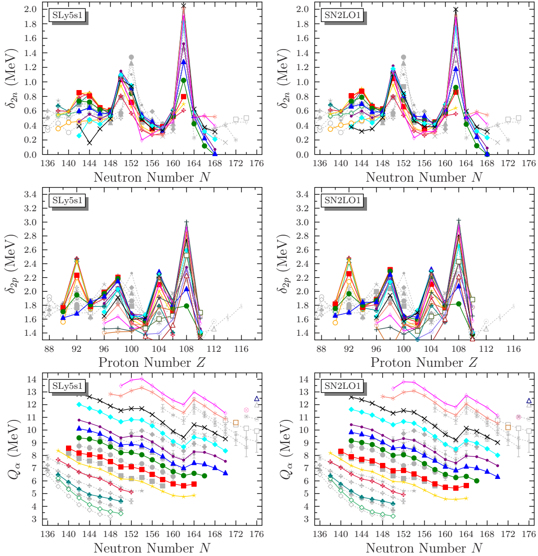


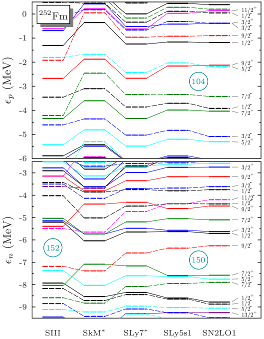


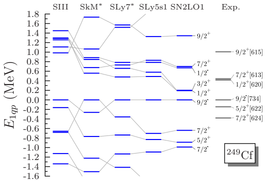


Ryssens and Bender, PRC 104 (2021) 044308

SN2LO1 applied to finite nuclei







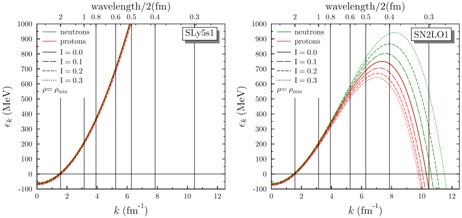
Bonnard, Ryssens, Bender, in preparation

Effective mass and dispersion relation in infinite matter

$$\epsilon_k = F_q^{1,1} + \left(\frac{\hbar^2}{2m_q} + F_q^{(\boldsymbol{\nabla},\boldsymbol{\nabla})} \right) \mathbf{k}^2 + \sum_\mu F_{q,\mu\mu}^{\nabla,\nabla} \, k_\mu^2 + F_q^{\Delta,\Delta} \, \mathbf{k}^4 \, .$$

The presence of the term proportional to $\mathbf{k}^4$ qualitatively changes the spectrum of eigenstates:

- At NLO, $\frac{\hbar^2}{2m_q} + F_q^{(\boldsymbol{\nabla},\boldsymbol{\nabla})}$ is always positive (around saturation at least, otherwise the isoscalar effective mass would be negative), such that $\lim_{k\to+\infty} \epsilon_k = +\infty$.
- At N2LO, the limit is determined by the sign of $F_q^{\Delta,\Delta}$, on which there is no direct constraint. Positive effective mass around saturation only requires that $F_q^{\Delta,\Delta}$ is "small" compared to $\hbar^2/2m_q$.
- For SN2LO1 $F_q^{\Delta,\Delta}$ is negative in symmetric matter, $\lim_{k\to+\infty} \epsilon_k = -\infty$
- The effective mass AT N2LO is k-dependent. Negative $F_q^{\Delta,\Delta}$ implies that the effective mass decreases with k and becomes negative at high k-values.



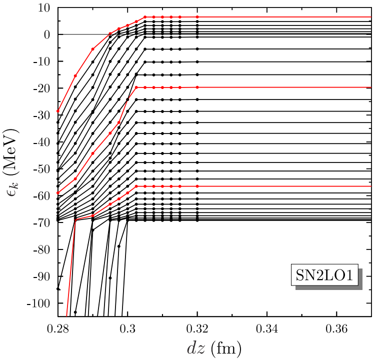
Wavelength

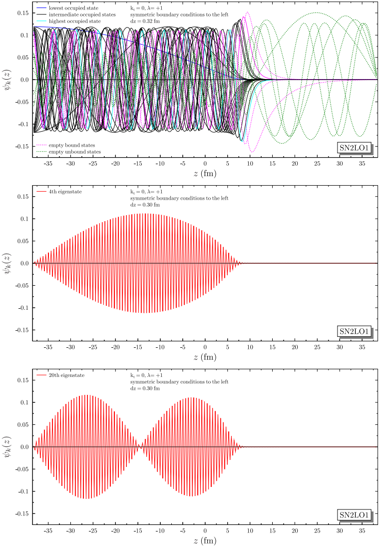
$$\lambda(k) = \frac{h}{p} = \frac{2\pi\hbar}{\hbar k} = \frac{2\pi}{k} \, ,$$

meaning a plane wave with k is resolved when dz is smaller than

$$dz_{\mathrm{max}} = \frac{\lambda}{2} = \frac{\pi}{k} \, .$$

Bender (unpublished)





Lowest 30 eigenvalues of one nucleon species in SINM as a function of stepsize dz.
The 10th, 20th, and 30th eigenstate are indicated in red.

Bender (unpublished)

Constructing the functional generator

$$\hat{\mathbf{k}}_{12} = -\tfrac{i}{2}(\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}_2) \qquad \text{incoming relative momentum}$$

$$\hat{\mathbf{k}}'_{12} = \tfrac{i}{2}(\boldsymbol{\nabla}'_1 - \boldsymbol{\nabla}'_2) \qquad \text{outgoing relative momentum}$$

$$\hat{\mathbf{q}}_{12} \equiv \hat{\mathbf{k}}_{12} - \hat{\mathbf{k}}'_{12} \qquad \text{momentum transfer}$$

$$\hat{\mathbf{Q}}_{12} \equiv \tfrac{1}{2}(\hat{\mathbf{k}}_{12} + \hat{\mathbf{k}}'_{12}) \qquad \text{average momentum}$$

For the construction of local densities and currents, it is useful to define the operators

$$\begin{aligned}
\hat{\mathbf{K}}_1 &\equiv -\mathrm{i}(\boldsymbol{\nabla}_1 + \boldsymbol{\nabla}'_1) \\
\hat{\mathbf{K}}_2 &\equiv -\mathrm{i}(\boldsymbol{\nabla}_2 + \boldsymbol{\nabla}'_2) \\
\hat{\mathbf{k}}_1 &\equiv -\tfrac{\mathrm{i}}{2}(\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}'_1) \\
\hat{\mathbf{k}}_2 &\equiv -\tfrac{\mathrm{i}}{2}(\boldsymbol{\nabla}_2 - \boldsymbol{\nabla}'_2) \\
k^{(2)}_{1,\mu\nu} &\equiv \tfrac{1}{2}\left(\nabla_{1,\mu}\nabla'_{1,\nu} + \nabla_{1,\nu}\nabla'_{1,\mu}\right) \\
k^{(2)}_{2,\mu\nu} &\equiv \tfrac{1}{2}\left(\nabla_{2,\mu}\nabla'_{2,\nu} + \nabla_{2,\nu}\nabla'_{2,\mu}\right)
\end{aligned}$$

$$\begin{aligned}
\hat{\mathbf{K}}_1\, \rho_q(\mathbf{r}_1, \mathbf{r}'_1)\Big|_{\mathbf{r}=\mathbf{r}'} &= -\mathrm{i}\boldsymbol{\nabla} D^{1,1}_q(\mathbf{r}) \\
\hat{\mathbf{k}}_1\, \rho_q(\mathbf{r}_1, \mathbf{r}'_1)\Big|_{\mathbf{r}=\mathbf{r}'} &= \mathbf{C}^{1,\nabla}_a(\mathbf{r}) \\
k^{(2)}_{1,\mu\nu}\, \rho_q(\mathbf{r}_1, \mathbf{r}'_1)\Big|_{\mathbf{r}=\mathbf{r}'} &= D^{\nabla,\nabla}_{q,\mu\nu}(\mathbf{r})
\end{aligned}$$

$$\begin{aligned}
\hat{\mathbf{q}}_{12} &= \hat{\mathbf{k}}_{12} - \hat{\mathbf{k}}'_{12} = \tfrac{1}{2}(\hat{\mathbf{K}}_1 - \hat{\mathbf{K}}_2) \\
\hat{\mathbf{Q}}_{12} &= \tfrac{1}{2}(\hat{\mathbf{k}}_{12} + \hat{\mathbf{k}}'_{12}) = \tfrac{1}{2}(\hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2)
\end{aligned}$$

$$\begin{aligned}
\hat{\mathbf{k}}_{12} &= -\tfrac{\mathrm{i}}{2}(\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}_2) = \hat{\mathbf{Q}}_{12} + \tfrac{1}{2}\hat{\mathbf{q}}_{12} = \tfrac{1}{2}(\hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2) + \tfrac{1}{4}(\hat{\mathbf{K}}_1 - \hat{\mathbf{K}}_2)\,, \\
\hat{\mathbf{k}}'_{12} &= +\tfrac{\mathrm{i}}{2}(\boldsymbol{\nabla}'_1 - \boldsymbol{\nabla}'_2) = \hat{\mathbf{Q}}_{12} - \tfrac{1}{2}\hat{\mathbf{q}}_{12} = \tfrac{1}{2}(\hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2) - \tfrac{1}{4}(\hat{\mathbf{K}}_1 - \hat{\mathbf{K}}_2)\,.
\end{aligned}$$

Bender and Proust, in preparation

operators in spin space

- the unit operator 1,
- the spin exchange operator

$$\hat{P}^{\sigma}_{12} \equiv \tfrac{1}{2}(1 + \hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2)$$

- the total spin operator (divided by $2\hbar$ to avoid having to keep track of these factors)

$$\hat{\mathbf{S}}_{12} \equiv \hat{\boldsymbol{\sigma}}_1 + \hat{\boldsymbol{\sigma}}_2 \,,$$

which is a pseudovector in coordinate space and a rank one tensor in the respective spin spaces of particles 1 and 2,
- the traceless rank-two tensor operator in spin space

$$\hat{S}^{(2)}_{12,\mu\nu} \equiv \tfrac{3}{2}\,\left(\hat{\sigma}_{1,\mu}\;\hat{\sigma}_{2,\nu} + \hat{\sigma}_{1,\nu}\;\hat{\sigma}_{2,\mu}\right) - \hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2\;\delta_{\mu\nu}\,.$$

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Operator structures that are even ($\eta = +1$) r odd ($\eta = -1$) under spatial exchange at NLO

momentum structures	rank	spin structures	η	gauge
$\mathbf{Q}^2 + \frac{1}{4}\mathbf{q}^2$	0	$\hat{\mathbb{1}}_{\sigma\otimes\sigma}$, $\hat{P}^{\sigma}_{12}$	$+1$	yes
$\mathbf{Q}^2 - \frac{1}{4}\mathbf{q}^2$	0	$\hat{\mathbb{1}}_{\sigma\otimes\sigma}$, $\hat{P}^{\sigma}_{12}$	-1	yes
$\mathbf{Q} \times \mathbf{q}$	1	$i\hat{\mathbf{S}}_{12}$	-1	yes
$Q_\mu Q_\nu + \frac{1}{4} q_\mu q_\nu$	2	$\hat{S}^{(2)}_{12,\mu\nu}$	$+1$	yes
$Q_\mu Q_\nu - \frac{1}{4} q_\mu q_\nu$	2	$\hat{S}^{(2)}_{12,\mu\nu}$	-1	yes

Operator structures that are even ($\eta = +1$) r odd ($\eta = -1$) under spatial exchange at N2LO

momentum structures	rank	spin structures	η	gauge
$\mathbf{Q}^4 + \frac{1}{16}\mathbf{q}^4$	0	$\hat{\mathbb{1}}_{\sigma\otimes\sigma}$, $\hat{P}^{\sigma}_{12}$	$+1$	yes
$\mathbf{Q}^4 - \frac{1}{16}\mathbf{q}^4$	0	$\hat{\mathbb{1}}_{\sigma\otimes\sigma}$, $\hat{P}^{\sigma}_{12}$	-1	yes
$\mathbf{Q}^2\mathbf{q}^2$	0	$\hat{\mathbb{1}}_{\sigma\otimes\sigma}$, $\hat{P}^{\sigma}_{12}$	$+1$	no
$(\mathbf{Q} \cdot \mathbf{q})^2$	0	$\hat{\mathbb{1}}_{\sigma\otimes\sigma}$, $\hat{P}^{\sigma}_{12}$	$+1$	no
$(\mathbf{Q}^2 + \frac{1}{4}\mathbf{q}^2)(\mathbf{Q} \times \mathbf{q})$	1	$i\hat{\mathbf{S}}_{12}$	-1	no
$(\mathbf{Q}^2 - \frac{1}{4}\mathbf{q}^2)(\mathbf{Q} \times \mathbf{q})$	1	$i\hat{\mathbf{S}}_{12}$	$+1$	no
$\mathbf{Q}^2 Q_\mu Q_\nu + \frac{1}{16}\mathbf{q}^2 q_\mu q_\nu$	2	$\hat{S}^{(2)}_{12,\mu\nu}$	$+1$	yes
$\mathbf{Q}^2 Q_\mu Q_\nu - \frac{1}{16}\mathbf{q}^2 q_\mu q_\nu$	2	$\hat{S}^{(2)}_{12,\mu\nu}$	-1	yes
$\mathbf{Q}^2 q_\mu q_\nu + \mathbf{q}^2 Q_\mu Q_\nu$	2	$\hat{S}^{(2)}_{12,\mu\nu}$	$+1$	no
$\mathbf{Q}^2 q_\mu q_\nu - \mathbf{q}^2 Q_\mu Q_\nu$	2	$\hat{S}^{(2)}_{12,\mu\nu}$	-1	no
$\frac{1}{2}(\mathbf{Q} \cdot \mathbf{q})(Q_\mu q_\nu + q_\mu Q_\nu)$	2	$\hat{S}^{(2)}_{12,\mu\nu}$	$+1$	no

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Recoupling of EDF generators to density generators

- When generating the EDF with the $\hat{Q}_{12,\mu}$ and $\hat{q}_{12,\nu}$ operators, one naturally arrives at an expression in terms of products of $(K_{1,\mu} - K_{2,\mu})$ and $(k_{1,\nu} - k_{2,\nu})$.
- Those containing $\hat{q}_{12,\nu} = \frac{1}{2}\,(K_{1,\mu} - K_{2,\mu})$ can be directly applied to density matrices when calculating the EDF. They just generate external derivatives of local densities.
- Those that contain more that one factor $(k_{1,\nu} - k_{2,\nu})$ cannot be directly applied, as multiple current generators $k_{1,\nu}$ acting on the same density matrix, do not yield an irreducible non-redundant hermitean local density. Instead, one recouples these operators to

$$k_\mu k_\nu = \frac{1}{4}\,K_\mu K_\nu + \frac{1}{2}\,(\nabla_\mu \nabla'_\nu + \nabla_\nu \nabla'_\mu) = \frac{1}{4}\,K_\mu K_\nu + \frac{1}{2}\,k^{(2)}_{\mu\nu}$$

Perlinska, Rohozinski, Dobaczewski, Nazarewicz, PRC 69 (2004) 014316]

- Similar (but more lengthy) relations hold for higher-order products $k_\mu k_\nu k_\kappa$ and $k_\mu k_\nu k_\kappa k_\lambda$.

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The central NLO terms

$$\mathbf{Q}^2 \pm \tfrac{1}{4}\mathbf{q}^2 \quad \rightarrow \quad \tfrac{1}{4}\,(\mathbf{k}_1 - \mathbf{k}_2)^2 \pm \tfrac{1}{16}\,(\mathbf{K}_1 - \mathbf{K}_2)^2 \rightarrow \tfrac{1}{2}\,k_2^{(2)} - \tfrac{1}{2}\,\mathbf{k}_1 \cdot \mathbf{k}_2 + \tfrac{1}{8}(1 \pm 2)\mathbf{K}_2^2$$

The central local N2LO terms

$$\begin{aligned} 2\mathbf{Q}^4 \pm \tfrac{1}{8}\mathbf{q}^4 \quad &\rightarrow \quad \tfrac{1}{8}\,(\mathbf{k}_1 - \mathbf{k}_2)^4 \pm \tfrac{1}{128}\,(\mathbf{K}_1 - \mathbf{K}_2)^4 \\ &\rightarrow \quad \tfrac{1}{4}\,k_2^{(4)} + \tfrac{1}{4}\,k_1^{(2)}k_2^{(2)} + \tfrac{1}{2}\,k_{1,\mu\nu}^{(2)}k_{2,\mu\nu}^{(2)} + \tfrac{1}{2}\,K_{2,\mu}K_{2,\nu}k_{2,\mu\nu}^{(2)} + \mathbf{k}_1 \cdot \mathbf{k}_2^{(3)} \\ &\qquad + \tfrac{1}{4}\mathbf{K}_2^2(\mathbf{k}_1 \cdot \mathbf{k}_2) - \tfrac{1}{2}(\mathbf{k}_1 \cdot \mathbf{K}_2)(\mathbf{K}_2 \cdot \mathbf{k}_2) + \tfrac{1}{16}(1 \pm 2)\mathbf{K}_2^4 \end{aligned}$$

One of the non-local central N2LO terms

$$(\mathbf{Q} \cdot \mathbf{q})^2 \rightarrow \tfrac{1}{16}[(\mathbf{K}_1 - \mathbf{K}_2) \cdot (\mathbf{k}_1 - \mathbf{k}_2)]^2 \quad \rightarrow \quad \tfrac{1}{2}\,K_{2,\mu}K_{2,\nu}k_{2,\mu\nu}^{(2)} - \tfrac{1}{2}(\mathbf{k}_1 \cdot \mathbf{K}_2)(\mathbf{K}_2 \cdot \mathbf{k}_2) + \tfrac{1}{8}\mathbf{K}_2^4 \tag{1}$$

And similar for the others.

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Central

$$\langle \mathrm{HF}|\hat{V}_i^{\mathrm{C}}|\mathrm{HF}\rangle = \langle \mathrm{HF}|t_i\,(1 + x_i \hat{P}_{12}^{\sigma})\,\hat{O}^{\pi}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_1',\mathbf{r}_2')|\mathrm{HF}\rangle$$

$$= \iiiint d^3r_1\; d^3r_2\; d^3r_1'\; d^3r_2'\; \hat{O}^{\pi}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2') \sum_{t=0,1} \Big[C_{c,i\pi}^{0,t}(i)\,\rho_t(\mathbf{r}_1,\mathbf{r}_1')\,\rho_t(\mathbf{r}_2,\mathbf{r}_2') + C_{c,i\pi}^{1,t}(t_i,x_i)\,\mathbf{s}_t(\mathbf{r}_1,\mathbf{r}_1')\cdot\mathbf{s}_t(\mathbf{r}_2,\mathbf{r}_2') \Big]$$

Spin-orbit

$$\langle \mathrm{HF}|\hat{V}_i^{\mathrm{LS}}|\mathrm{HF}\rangle = \langle \mathrm{HF}|W_i\,\hat{\mathbf{S}}_{12}\cdot\hat{\mathbf{O}}^{\pi}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_1',\mathbf{r}_2')|\mathrm{HF}\rangle$$

$$= \iiiint d^3r_1\; d^3r_2\; d^3r_1'\; d^3r_2' \sum_{t=0,1} C_{so,i\pi}^{1t}(W_i)\,\hat{\mathbf{O}}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2')\cdot\big[\mathbf{s}_t(\mathbf{r}_1,\mathbf{r}_1')\,\rho_t(\mathbf{r}_2,\mathbf{r}_2') + \rho_t(\mathbf{r}_1,\mathbf{r}_1')\,\mathbf{s}_t(\mathbf{r}_2,\mathbf{r}_2')\big)$$

Tensor

$$\langle \mathrm{HF}|\hat{V}_i^{\mathrm{T}}|\mathrm{HF}\rangle = \langle \mathrm{HF}|\hat{S}_{\mu\nu}^{(2)}\,\hat{O}_{\mu\nu}^{\pi}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_1',\mathbf{r}_2')|\mathrm{HF}\rangle$$

$$= \iiiint d^3r_1\; d^3r_2\; d^3r_1'\; d^3r_2' \sum_{t=0,1} C_{t,i\pi}^{1t}(W_i)\,\hat{O}_{\mu\nu}^{\pi}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_1',\mathbf{r}_2')\Big[\tfrac{3}{2}\,s_{0,\mu}(\mathbf{r}_1,\mathbf{r}_1')\,s_{0,\nu}(\mathbf{r}_2,\mathbf{r}_2') + \tfrac{3}{2}\,s_{0,\nu}(\mathbf{r}_1,\mathbf{r}_1')\,s_{0,\mu}(\mathbf{r}_2,\mathbf{r}_2') - \mathbf{s}_0(\mathbf{r}_1,\mathbf{r}_1')\cdot\mathbf{s}_0(\mathbf{r}_2,\mathbf{r}_2')\,\delta_{\mu\nu}\Big]$$

Bender and Proust, in preparation

Coupling constants of the LO and NLO terms in the EDF. Terms containing spin densities $D^{A,B\sigma}$ are multiplied by generic coupling constants with $s = 1$, whereas terms not containing spin densities are multiplied by generic coupling constants with $s = 0$.

term		$C^{s,t}_{c,0+}$
$D^{1,1}_t D^{1,1}_t$	$A^{(0,1)}_{t,\mathrm{e}} =$	1
$\mathbf{D}^{1,\sigma}_t \cdot \mathbf{D}^{1,\sigma}_t$	$A^{(0,1)}_{t,\mathrm{o}} =$	1

term		$C^{s,t}_{c,1+}$	$C^{s,t}_{c,2-}$	$C^{s,t}_{t,1+}$	$C^{s,t}_{t,2-}$
$D^{1,1}_t \, D^{(\nabla,\nabla)}_t$	$A^{(2,2)}_{t,\mathrm{e}} =$	$+\frac{1}{2}$	$+\frac{1}{2}$		
$D^{1,1}_t (\Delta D^{1,1}_t)$	$A^{(2,1)}_{t,\mathrm{e}} =$	$-\frac{3}{8}$	$+\frac{1}{8}$		
$C^{1,\nabla\sigma}_{t,\mu\nu} \, C^{1,\nabla\sigma}_{t,\mu\nu}$	$A^{(2,3)}_{t,\mathrm{e}} =$	$-\frac{1}{2}$	$-\frac{1}{2}$	$+\frac{1}{2}$	$+\frac{1}{2}$
$C^{1,\nabla\sigma}_{t,\mu\nu} \, C^{1,\nabla\sigma}_{t,\nu\mu}$	$A^{(2,X)}_{t,\mathrm{e}} =$			$-\frac{3}{4}$	$-\frac{3}{4}$
$C^{1,(\nabla\sigma)}_t \, C^{1,(\nabla\sigma)}_t$	$A^{(2,X)}_{t,\mathrm{e}} =$			$-\frac{3}{4}$	$-\frac{3}{4}$
$\mathbf{D}^{1,\sigma}_t \cdot \mathbf{D}^{\nabla,(\nabla\sigma)}_t$	$A^{(2,X)}_{t,\mathrm{o}} =$			$+\frac{3}{2}$	$+\frac{3}{2}$
$\mathbf{D}^{1,\sigma}_t \cdot \mathbf{D}^{(\nabla,\nabla)\sigma}_t$	$A^{(2,2)}_{t,\mathrm{o}} =$	$+\frac{1}{2}$	$+\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$
$\mathbf{D}^{1,\sigma}_t \cdot (\Delta \mathbf{D}^{1,\sigma}_t)$	$A^{(2,1)}_{t,\mathrm{o}} =$	$-\frac{3}{8}$	$+\frac{1}{8}$	$+\frac{3}{8}$	$-\frac{1}{8}$
$(\boldsymbol{\nabla} \cdot \mathbf{D}^{1,\sigma}_t)(\boldsymbol{\nabla} \cdot \mathbf{D}^{1,\sigma}_t)$	$A^{(2,X)}_{t,\mathrm{o}} =$			$+\frac{9}{8}$	$-\frac{3}{8}$
$\mathbf{C}^{1,\nabla}_t \cdot \mathbf{C}^{1,\nabla}_t$	$A^{(2,3)}_{t,\mathrm{o}} =$	$-\frac{1}{2}$	$-\frac{1}{2}$		

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terms	$C^{s,t}_{c,1(4)+}$	$C^{s,t}_{c,2(4)-}$	$C^{s,t}_{c,3(4)+}$	$C^{s,t}_{c,4(4)+}$	$C^{s,t}_{t,1(4)+}$	$C^{s,t}_{t,2(4)-}$	$C^{s,t}_{t,3(4)+}$	$C^{s,t}_{t,4(4)-}$	$C^{s,t}_{t,5(4)+}$
$D^{1,1}_t \, D^{\Delta,\Delta}_t$	$+\frac{1}{4}$	$+\frac{1}{4}$							
$D^{(\nabla,\nabla)}_t \, D^{(\nabla,\nabla)}_t$	$+\frac{1}{4}$	$+\frac{1}{4}$							
$D^{\nabla,\nabla}_{t,\mu\nu} \, D^{\nabla,\nabla}_{t,\mu\nu}$	$+\frac{1}{2}$	$+\frac{1}{2}$							
$D^{1,1}_t \, (\nabla_\mu \nabla_\nu D^{\nabla,\nabla}_{t,\mu\nu})$	$-\frac{1}{2}$	$-\frac{1}{2}$		$-\frac{1}{2}$					
$D^{(\nabla,\nabla)}_t \, (\Delta D^{1,1}_t)$			$-\frac{1}{2}$						
$(\Delta D^{1,1}_t)(\Delta D^{1,1}_t)$	$+\frac{3}{16}$	$-\frac{1}{16}$	$+\frac{1}{8}$	$+\frac{1}{8}$					
$C^{1,\nabla\sigma}_{t,\mu\nu} \, C^{\Delta,\nabla\sigma}_{t,\mu\nu}$	$+1$	$+1$			-1	-1			
$C^{1,\nabla\sigma}_{t,\mu\nu} \, C^{\Delta,\nabla\sigma}_{t,\nu\mu}$					$+\frac{3}{4}$	$+\frac{3}{4}$			
$C^{1,(\nabla\sigma)}_t \, C^{\Delta,(\nabla\sigma)}_t$					$+\frac{3}{4}$	$+\frac{3}{4}$			
$C^{1,\nabla\sigma}_{t,\mu\nu} \, C^{\nabla\nabla,(\nabla\sigma)}_{t,\mu\nu}$					$+\frac{3}{2}$	$+\frac{3}{2}$			
$C^{1,\nabla\sigma}_{t,\mu\nu} \, (\Delta C^{1,\nabla\sigma}_{t,\mu\nu})$	$-\frac{1}{4}$	$-\frac{1}{4}$	$+\frac{1}{2}$		$+\frac{1}{4}$	$+\frac{1}{4}$	$-\frac{1}{2}$		
$C^{1,\nabla\sigma}_{t,\mu\nu} \, (\Delta C^{1,\nabla\sigma}_{t,\nu\mu})$					$-\frac{3}{16}$	$-\frac{3}{16}$	$+\frac{3}{8}$	$+\frac{3}{8}$	
$C^{1,(\nabla\sigma)}_t \, (\Delta C^{1,(\nabla\sigma)}_t)$					$-\frac{3}{16}$	$-\frac{3}{16}$	$+\frac{3}{8}$	$+\frac{3}{8}$	
$(\nabla_\mu C^{1,\nabla\sigma}_{t,\mu\nu})(\nabla_\kappa C^{1,\nabla\sigma}_{t,\kappa\nu})$	$-\frac{1}{2}$	$-\frac{1}{2}$		$-\frac{1}{2}$	$+\frac{1}{2}$	$+\frac{1}{2}$			$+\frac{1}{2}$
$(\nabla_\nu C^{1,\nabla\sigma}_{t,\mu\nu})(\nabla_\kappa C^{1,\nabla\sigma}_{t,\mu\kappa})$					$-\frac{3}{8}$	$-\frac{3}{8}$	$-\frac{3}{4}$	$+\frac{3}{4}$	
$(\nabla_\nu C^{1,\nabla\sigma}_{t,\mu\nu})(\nabla_\kappa C^{1,\nabla\sigma}_{t,\kappa\mu})$					$-\frac{3}{4}$	$-\frac{3}{4}$			$-\frac{3}{4}$
$C^{1,(\nabla\sigma)}_t \, (\nabla_\mu \nabla_\nu C^{1,\nabla\sigma}_{t,\mu\nu})$									$+\frac{3}{4}$

terms	$C^{s,t}_{c,1(4)+}$	$C^{s,t}_{c,2(4)-}$	$C^{s,t}_{c,3(4)+}$	$C^{s,t}_{c,4(4)+}$	$C^{s,t}_{t,1(4)+}$	$C^{s,t}_{t,2(4)-}$	$C^{s,t}_{t,3(4)+}$	$C^{s,t}_{t,4(4)-}$	$C^{s,t}_{t,5(4)+}$
$\mathbf{D}^{1,\sigma}_t \cdot \mathbf{D}^{\Delta,\Delta\sigma}_t$	$+\frac{1}{4}$	$+\frac{1}{4}$			$-\frac{1}{4}$	$-\frac{1}{4}$			
$\mathbf{D}^{1,\sigma}_t \cdot \mathbf{D}^{\Delta,\nabla(\nabla\sigma)}_t$					$+\frac{3}{4}$	$+\frac{3}{4}$			
$\mathbf{D}^{(\nabla,\nabla)\sigma}_t \cdot \mathbf{D}^{(\nabla,\nabla)\sigma}_t$	$+\frac{1}{4}$	$+\frac{1}{4}$			$-\frac{1}{4}$	$-\frac{1}{4}$			
$\mathbf{D}^{(\nabla,\nabla)\sigma}_t \cdot \mathbf{D}^{\nabla,(\nabla\sigma)}_t$					$+\frac{3}{4}$	$+\frac{3}{4}$			
$\mathbf{D}^{\nabla,(\nabla\sigma)}_t \cdot \mathbf{D}^{\nabla,(\nabla\sigma)}_t$					$+\frac{3}{4}$	$+\frac{3}{4}$			
$D^{\nabla,\nabla\sigma}_{t,\mu\nu\kappa}\, D^{\nabla,\nabla\sigma}_{t,\mu\nu\kappa}$	$+\frac{1}{2}$	$+\frac{1}{2}$			$-\frac{1}{2}$	$-\frac{1}{2}$			
$D^{\nabla,\nabla\sigma}_{t,\mu\nu\kappa}\, D^{\nabla,\nabla\sigma}_{t,\kappa\mu\nu}$					$+\frac{3}{4}$	$+\frac{3}{4}$			
$\mathbf{D}^{(\nabla,\nabla)\sigma}_t \cdot (\Delta\mathbf{D}^{1,\sigma}_t)$			$-\frac{1}{2}$				$+\frac{1}{2}$		
$\mathbf{D}^{\nabla,(\nabla\sigma)}_t \cdot (\Delta\mathbf{D}^{1,\sigma}_t)$							$-\frac{3}{4}$	$-\frac{3}{4}$	
$(\boldsymbol{\nabla} \cdot \mathbf{D}^{1,\sigma}_t)(\boldsymbol{\nabla} \cdot \mathbf{D}^{(\nabla,\nabla)\sigma}_t)$							$+\frac{3}{4}$	$-\frac{3}{4}$	
$(\boldsymbol{\nabla} \cdot \mathbf{D}^{1,\sigma}_t)(\boldsymbol{\nabla} \cdot \mathbf{D}^{\nabla,(\nabla\sigma)}_t)$					$+\frac{3}{4}$	$+\frac{3}{4}$			$+\frac{3}{4}$
$D^{1,\sigma}_{t,\kappa}\,(\nabla_\mu \nabla_\nu D^{\nabla,\nabla\sigma}_{t,\mu\nu\kappa})$	$-\frac{1}{2}$	$-\frac{1}{2}$		$-\frac{1}{2}$	$+\frac{1}{2}$	$+\frac{1}{2}$			$+\frac{1}{2}$
$D^{1,\sigma}_{t,\kappa}\,(\nabla_\mu \nabla_\nu D^{\nabla,\nabla\sigma}_{t,\kappa\mu\nu})$					$-\frac{3}{4}$	$-\frac{3}{4}$			$-\frac{3}{4}$
$(\Delta\mathbf{D}^{1,\sigma}_t) \cdot (\Delta\mathbf{D}^{1,\sigma}_t)$	$+\frac{3}{16}$	$-\frac{1}{16}$	$+\frac{1}{8}$	$+\frac{1}{8}$	$-\frac{3}{16}$	$+\frac{1}{16}$	$-\frac{1}{8}$		$-\frac{1}{8}$
$(\boldsymbol{\nabla} \cdot \mathbf{D}^{1,\sigma}_t)(\Delta\, \boldsymbol{\nabla} \cdot \mathbf{D}^{1,\sigma}_t)$					$-\frac{9}{16}$	$+\frac{3}{16}$	$-\frac{3}{8}$		$-\frac{3}{8}$
$\mathbf{C}^{1,\nabla}_t \cdot \mathbf{C}^{\Delta,\nabla}_t$	$+1$	$+1$							
$\mathbf{C}^{1,\nabla}_t \cdot (\Delta\mathbf{C}^{1,\nabla}_t)$	$-\frac{1}{4}$	$-\frac{1}{4}$	$+\frac{1}{2}$						
$(\boldsymbol{\nabla} \cdot \mathbf{C}^{1,\nabla}_t)(\boldsymbol{\nabla} \cdot \mathbf{C}^{1,\nabla}_t)$	$-\frac{1}{2}$	$-\frac{1}{2}$		$-\frac{1}{2}$					

Bender and Proust, in preparation

term		$C^{s,t}_{so,0-}$
$D^{1,1}_t \, (\boldsymbol{\nabla} \cdot \mathbf{C}^{1,\nabla\times\sigma}_t)$	$A^{(2,4)}_{t,\mathrm{e}} =$	-1
$\mathbf{D}^{1,\sigma}_t \cdot (\boldsymbol{\nabla} \times \mathbf{C}^{1,\nabla}_t)$	$A^{(2,4)}_{t,\mathrm{o}} =$	-1

terms		$C^{s,t}_{so,1+}$	$C^{s,t}_{so,2-}$
$D^{1,1}_t \, (\boldsymbol{\nabla} \cdot \mathbf{C}^{\Delta,\nabla\times\sigma}_t)$	$A^{(4,X)}_{t,\mathrm{e}} =$	$+\frac{1}{4}$	$+\frac{1}{4}$
$D^{(\nabla,\nabla)}_t \, (\boldsymbol{\nabla} \cdot \mathbf{C}^{1,\nabla\times\sigma}_t)$	$A^{(4,X)}_{t,\mathrm{e}} =$	$-\frac{1}{4}$	$-\frac{1}{4}$
$(\Delta D^{1,1}_t)(\boldsymbol{\nabla} \cdot \mathbf{C}^{1,\nabla\times\sigma}_t)$	$A^{(4,X)}_{t,\mathrm{e}} =$	$-\frac{1}{4}$	$+\frac{1}{4}$
$\epsilon_{\mu\nu\kappa} \, D^{\nabla,\nabla}_{t,\alpha\mu} \, (\nabla_\nu C^{1,\nabla\sigma}_{t,\alpha\kappa})$	$A^{(4,X)}_{t,\mathrm{e}} =$	$+\frac{1}{2}$	$+\frac{1}{2}$
$\mathbf{D}^{1,\sigma}_t \cdot (\boldsymbol{\nabla} \times \mathbf{C}^{\Delta,\nabla}_t)$	$A^{(4,X)}_{t,\mathrm{o}} =$	$+\frac{1}{4}$	$+\frac{1}{4}$
$\mathbf{D}^{(\nabla,\nabla)\sigma}_t \cdot (\boldsymbol{\nabla} \times \mathbf{C}^{1,\nabla}_t)$	$A^{(4,X)}_{t,\mathrm{o}} =$	$-\frac{1}{4}$	$-\frac{1}{4}$
$(\Delta \mathbf{D}^{1,\sigma}_t) \cdot (\boldsymbol{\nabla} \times \mathbf{C}^{1,\nabla}_t)$	$A^{(4,X)}_{t,\mathrm{o}} =$	$-\frac{1}{4}$	$+\frac{1}{4}$
$D^{\nabla,\nabla\times\sigma}_{t,\mu\nu} \, (\nabla_\nu C^{1,\nabla}_{t,\mu})$	$A^{(4,X)}_{t,\mathrm{o}} =$	$-\frac{1}{2}$	$-\frac{1}{2}$

New spherical coordinate-space HFB code

Ansatz for single-particle state

$$\Psi_{\alpha j_\alpha \ell_\alpha m}(\mathbf{r}) \equiv \Psi_{\alpha m}(\mathbf{r}) = \sqrt{4\pi}\,\psi_\alpha(r)\,\Omega_{j_\alpha \ell_\alpha m}(\vartheta,\varphi)$$

with the spinor spherical harmonics

$$\Omega_{j\ell m}(\vartheta,\varphi) = \sum_{m_\ell m_s} (\ell\, m_\ell\, \tfrac{1}{2}\, m_s \,|\, j\, m)\, \mathrm{Y}_{\ell m_\ell}(\vartheta,\varphi)\,\chi_{m_s} = \begin{pmatrix} \left(\ell\,\tfrac{1}{2}\,j\middle| m-\tfrac{1}{2}\,\tfrac{1}{2}\,m\right)\mathrm{Y}_{\ell\,m-\frac{1}{2}}(\vartheta,\varphi) \\ \left(\ell\,\tfrac{1}{2}\,j\middle| m+\tfrac{1}{2}\,-\tfrac{1}{2}\,m\right)\mathrm{Y}_{\ell\,m+\frac{1}{2}}(\vartheta,\varphi) \end{pmatrix}.$$

for which holds

$$\sum_{m=-j}^{j} \Omega^\dagger_{j\ell m}(\vartheta',\varphi')\,\Omega_{j\ell m}(\vartheta,\varphi) = \frac{2j+1}{4\pi}\,P_\ell(\mathbf{e}_{r'}\cdot\mathbf{e}_r)$$

Represent all spatial functions as cartesian tensors proportional to the unit tensors

$$E^{(0)} = \mathbf{e}_r\cdot\mathbf{e}_r = \frac{\mathbf{r}\cdot\mathbf{e}_r}{r^2} = \frac{r^2}{r^2} = 1\,, \qquad E^{(1)}_\mu = \mathbf{e}_r\cdot\mathbf{e}_\mu = \frac{\mathbf{r}\cdot\mathbf{e}_\mu}{r} = \frac{r_\mu}{r}\,,$$

$$E^{(0)}_{\mu\nu} = \tfrac{1}{3}\,\delta_{\mu\nu}\,\mathbf{e}_r\cdot\mathbf{e}_r = \tfrac{1}{3}\,\delta_{\mu\nu}\,, \qquad E^{(2)}_{\mu\nu} = \frac{\mathbf{r}\cdot\mathbf{e}_\mu}{r}\,\frac{\mathbf{r}\cdot\mathbf{e}_\nu}{r} - \tfrac{1}{3}\delta_{\mu\nu} = \frac{r_\mu\, r_\nu}{r^2} - \tfrac{1}{3}\delta_{\mu\nu}$$

where $\mathbf{e}_\mu$ are unit vectors in the cartesian directions x, y, z. All local functions have a structure that is a radial function times an elementary tensor

$S(\mathbf{r}) = S(r)$	scalar
$V_\mu(\mathbf{r}) = V_r(r)\,\dfrac{r_\mu}{r}$	vector
$T^{(0)}_{\mu\nu}(\mathbf{r}) = T^{(0)}(r)\,E^{(0)}_{\mu\nu}$	isotropic rank-2 tensor
$T^{(2)}_{\mu\nu}(\mathbf{r}) = T^{(2)}(r)\,E^{(2)}_{\mu\nu}$	symmetric traceless rank-2 tensor

With that all local densities and the single-particle Hamiltonian can be constructed *without using angular-momentum coupling*.

Bender, in preparation

The non-vanishing densities in spherical symmetry are

$$D^{1,1}(r) = \sum_{\alpha} (2j_\alpha + 1)\, \rho_{\alpha\alpha}\, |\psi_\alpha(r)|^2 ,$$

$$D^{(\nabla,\nabla)}(r) = \sum_{\alpha} (2j_\alpha + 1)\, \rho_{\alpha\alpha} \left\{ \Big|[\partial_r\, \psi_\alpha(r)]\Big|^2 + \frac{\ell(\ell+1)}{r^2}\, |\psi_\alpha(r)|^2 \right\} ,$$

$$D^{\nabla,\nabla}_{\mu\nu}(r) = \sum_{\alpha} (2j_\alpha + 1)\, \rho_{\alpha\alpha} \left\{ \Big|[\partial_r\, \psi_\alpha(r)]\Big|^2 + \frac{\ell(\ell+1)}{r^2}\, |\psi_\alpha(r)|^2 \right\} E^{(0)}_{\mu\nu}$$
$$+ \sum_{\alpha} (2j_\alpha + 1)\, \rho_{\alpha\alpha} \left\{ \Big|[\partial_r\, \psi_\alpha(r)]\Big|^2 - \frac{1}{2}\frac{\ell(\ell+1)}{r^2}\, |\psi_\alpha(r)|^2 \right\} E^{(2)}_{\mu\nu} ,$$

$$D^{\Delta,\Delta}_{q}(r) = \sum_{\alpha} (2j_\alpha + 1)\, \rho_{\alpha\alpha} \left| \left[\left(\Delta_r - \frac{\ell(\ell+1)}{r^2} \right) \psi_\alpha(r) \right] \right|^2 ,$$

$$C^{1,(\boldsymbol{\nabla}\times\boldsymbol{\sigma})}_{q,r}(r) = \sum_{\alpha} (2j_\alpha + 1)\, \rho_{\alpha\alpha}\, \frac{\langle \ell\sigma \rangle_\alpha}{r}\, |\psi_\alpha(r)|^2 ,$$

$$C^{\Delta,(\boldsymbol{\nabla}\times\boldsymbol{\sigma})}_{q,r}(r) = \sum_{\alpha} (2j_\alpha + 1)\, \rho_{\alpha\alpha}\, \frac{\langle \ell\sigma \rangle_\alpha}{2R} \left\{ \psi^*_\alpha(r) \left[\left(\Delta_r - \frac{\ell(\ell+1)}{r^2} \right) \psi_\alpha(r) \right] + \left[\left(\Delta_r - \frac{\ell(\ell+1)}{r^2} \right) \psi^*_\alpha(r) \right] \psi_\alpha(r) \right\}$$

with

$$\langle \ell\sigma \rangle_\alpha = \left[j_\alpha(j_\alpha+1) - \ell_\alpha(\ell_\alpha+1) - \tfrac{3}{4} \right]$$

The choice of computationally-friendly densities for Cartesian 3D also leads to a simple form of the densities in spherical symmetry.

Bender, in preparation

$$
\begin{aligned}
\hat{h}_q \psi_\alpha(r) = \bigg\{ & - \frac{\hbar^2}{2m} \Big[\Delta_r - \frac{\ell_\alpha(\ell_\alpha+1)}{r^2} \Big] \\
& + F_q^{1,1}(r) \\
& + \Big[j_\alpha(j_\alpha+1) - \ell_\alpha(\ell_\alpha+1) - \tfrac{3}{4} \Big] \, \tfrac{1}{r} \, G_{r,q}^{1,(\nabla\times\sigma)}(r) \\
& - \big[\partial_r F_q^{(\nabla,\nabla)}(r) \big] \, \partial_r - F_q^{(\nabla,\nabla)}(r) \Big[\Delta_r - \frac{\ell_\alpha(\ell_\alpha+1)}{r^2} \Big] \\
& - \Big\{ \partial_r \, [F^{\nabla,\nabla}]_q^{(0)}(r) \Big\} \, \partial_r - [F^{\nabla,\nabla}]_q^{(0)}(r) \Big[\Delta_r - \frac{\ell_\alpha(\ell_\alpha+1)}{r^2} \Big] \\
& - \Big\{ \partial_r \, [F^{\nabla,\nabla}]_q^{(2)}(r) \Big\} \, \partial_r - [F^{\nabla,\nabla}]_q^{(2)}(r) \Big[\Delta_r + \frac{1}{2} \, \frac{\ell_\alpha(\ell_\alpha+1)}{r^2} \Big] \\
& + \tfrac{1}{2} \Big[j_\alpha(j_\alpha+1) - \ell_\alpha(\ell_\alpha+1) - \tfrac{3}{4} \Big] \Big[\Delta_r - \frac{\ell_\alpha(\ell_\alpha+1)}{r^2} \Big] \, \tfrac{1}{r} \, G_{q,r}^{\Delta,(\nabla\times\sigma)}(r) \\
& + \tfrac{1}{2} \Big[j_\alpha(j_\alpha+1) - \ell_\alpha(\ell_\alpha+1) - \tfrac{3}{4} \Big] \, \tfrac{1}{r} \, G_{q,r}^{\Delta,(\nabla\times\sigma)}(r) \Big[\Delta_r - \frac{\ell_\alpha(\ell_\alpha+1)}{r^2} \Big] \\
& + \Big[\Delta_r - \frac{\ell_\alpha(\ell_\alpha+1)}{r^2} \Big] \, F_q^{(\Delta,\Delta)}(r) \Big[\Delta_r - \frac{\ell_\alpha(\ell_\alpha+1)}{r^2} \Big] \bigg\} \, \psi_\alpha(r) \, .
\end{aligned}
$$

The new operator structure introduce additional dependences on orbital angular momentum ℓ of kinetic and spin-orbit terms.

Bender, in preparation

The single-particle Hamiltonian is represented as a matrix in coordinate space that acts on reduced wave functions $\phi_\alpha(r) = r\,\psi_\alpha(r)$, where derivatives are represented as Lagrange-mesh derivatives $D^{(2)}_{ij}$ in coordinate space

$$
\begin{aligned}
h_{ij} = & -\frac{\hbar^2}{2m}\,D^{(2)}_{ij} + \frac{\hbar^2}{2m}\,\frac{\ell_\alpha(\ell_\alpha+1)}{r_i^2}\,\delta_{ij} \\
& + F^{1,1}_{q,i}\,\delta_{ij} \\
& + G^{1,(\nabla\times\sigma)}_{r,q,i}\,\frac{\langle\ell\sigma\rangle_\alpha}{r_i}\,\delta_{ij} \\
& - \tfrac{1}{2}\,D^{(2)}_{ij}\,F^{(\nabla,\nabla)}_{q,j} - \tfrac{1}{2}\,F^{(\nabla,\nabla)}_{q,i}\,D^{(2)}_{ij} + \tfrac{1}{2}\,\big[\Delta_r F^{(\nabla,\nabla)}_q\big]_i\,\delta_{ij} + F^{(\nabla,\nabla)}_{q,i}\,\frac{\ell_\alpha(\ell_\alpha+1)}{r_i^2}\,\delta_{ij} \\
& - \tfrac{1}{2}\,D^{(2)}_{ij}\,\big[F^{(\nabla,\nabla)}\big]^{(0)}_{q,j} - \tfrac{1}{2}\,\big[F^{(\nabla,\nabla)}\big]^{(0)}_{q,i}\,D^{(2)}_{ij} + \tfrac{1}{2}\,\Big\{\Delta_r\big[F^{(\nabla,\nabla)}\big]^{(0)}_q\Big\}_i\,\delta_{ij} + \big[F^{(\nabla,\nabla)}\big]^{(0)}_{q,i}\,\frac{\ell_\alpha(\ell_\alpha+1)}{r_i^2}\,\delta_{ij} \\
& - \tfrac{1}{2}\,D^{(2)}_{ij}\,\big[F^{(\nabla,\nabla)}\big]^{(2)}_{q,j} - \tfrac{1}{2}\,\big[F^{(\nabla,\nabla)}\big]^{(2)}_{q,i}\,D^{(2)}_{ij} + \tfrac{1}{2}\,\Big\{\Delta_r\big[F^{(\nabla,\nabla)}\big]^{(2)}_q\Big\}_i\,\delta_{ij} - \tfrac{1}{2}\,\big[F^{(\nabla,\nabla)}\big]^{(2)}_{q,i}\,\frac{\ell_\alpha(\ell_\alpha+1)}{r_i^2}\,\delta_{ij} \\
& + \sum_k D^{(2)}_{ik}\,F^{(\Delta,\Delta)}_{q,k}\,D^{(2)}_{kj} - D^{(2)}_{ij}\,\frac{\ell_\alpha(\ell_\alpha+1)}{r_j^2} - \frac{\ell_\alpha(\ell_\alpha+1)}{r_i^2}\,D^{(2)}_{ij} + F^{(\Delta,\Delta)}_{q,i}\,\frac{\ell_\alpha^2(\ell_\alpha+1)^2}{r_i^4}\,\delta_{ij} \\
& + \tfrac{1}{2}\,D^{(2)}_{ij}\,G^{\Delta,(\nabla\times\sigma)}_{q,r,j}\,\frac{\langle\ell\sigma\rangle_\alpha}{r_j} + \tfrac{1}{2}\,G^{\Delta,(\nabla\times\sigma)}_{q,r,i}\,\frac{\langle\ell\sigma\rangle_\alpha}{r_i}\,D^{(2)}_{ij} - G^{\Delta,(\nabla\times\sigma)}_{q,r,i}\,\frac{\langle\ell\sigma\rangle_\alpha}{r_i}\,\frac{\ell_\alpha(\ell_\alpha+1)}{r_i^2}\,\delta_{ij} \\
= & \; h_{ji}\,.
\end{aligned}
$$

The first derivatives (that are not symmetric matrices on the radial mesh) are substituted with (the symmetric matrices) of second derivatives to ensure that the matrix h_{ji} can be diagonalised with standard matrix techniques (Hooverman, NPA 189 (1972) 155)

Bender, in preparation

- implementation in MOCCa will be taken care of by hephaestos (see talk by W. Ryssens)

  Ryssens, work in progress

- Newly designed spherical coordinate-space code (see previous slides)
- Newly designed semi-infinite matter HF code (see previous slides) that can handle arbitrary asymmetries up to the drip line
- (symmetric) semi-infinite matter calculation in ETF(2)-Fermi designed to handle N2LO EDFs - solving traditional ETF would become a complicated self-consistent problem so one needs an additional approximation to bring it back to the computational simplicity of ETF(4) for NLO EDFs.

  Proust, Lallouet, Davesne, Meyer, PRC 106 (2022) 054321

- Completely rewritten code for parameter adjustment

  Bonnard, Bender, Bennaceur (unpublished)

- N2LO offers new degrees of freedom
  - effective mass becomes momentum dependent in matter
  - The N2LO kinetic terms dominate the single-particle energy at high k, and, when used with a standard density dependence, it also dominates E/A at high density.
  - higher-order angular-momentum-dependent contributions to the potential, effective mass, spin-orbit potential in nuclei that depend on orbital angular momentum
  - direction dependent effective mass in finite nuclei (and anisotropic nuclear matter)
  - non-local terms that only act on the surface, not in bulk matter, and (probably) impact the the transport of nucleons in the nucleus
  - generalized spin-orbit interaction

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