Building the UNEDF from the ground up

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Technical Details:

The density matrix expansion (DME) can be used to build a UNEDF that is directly linked to underlying two- and three-nucleon interactions and microscopic many-body theory, in contrast to purely empirical Skyrme functionals. However, the original DME of Negele and Vautherin (and subsequent variations thereof) performs very poorly in describing the non-local spin-vector part of the density matrix. This is a severe limitation since it means that spin-orbit properties are poorly described by the conventional DME.

In Ref. 1, the failings of the conventional DME were traced to the neglect of two key features found in most finite fermi systems: 1) diffusivity of the local momentum distribution and 2) anisotropy of the local momentum distribution. Both of these effects are most pronounced at the nuclear surface, and must be accounted for if the DME is to provide an accurate description of spin-orbit properties (the spin-vector part of the density matrix is a surface-peaked quantity). In Ref.1, a new variant of the DME was formulated (the "PI-DME") that incorporates these two surface effects resulting in a substantially improved description of the spin-vector part of the density matrix.

References:
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1) B. Gebremariam, T. Duguet and S.K. Bogner, "An improved density matrix expansion for spin-unsaturated nuclei", arXiv:0910.4979.
2) B. Gebremariam, S.K. Bogner and T. Duguet, "Symbolic computation of the Hartree-Fock energy from a chiral EFT 3N interaction at NNLO", arXiv:0912.3086.

Explanation of the pictures:

• The plot in the upper left hand corner shows the anisotropy of the the local momentum distribution calculated for Cr isotopes. This anisotropy is most pronounced in the surface region. The behaviour is universal in all isotope chains we've looked at (I.e., crossover from oblate to prolate at the surface). Earlier implementations of the DME ignored this anisotropy, which has severe consequences for the spin-vector part of the density matrix due to its surface-peaked character.

- The plots at the bottom show the large improvement over the original Negele and Vautherin (NVDME) version of the DME for the Cr and Pb isotope chains when this anisotropy is incorporated into the improved PI-DME. The quantity being plotted is the HF energy involving the non-local spin densities $S(r_1,r_2)V(r_1-r_2)S(r_2,r_1)$. In this example, the interaction is one pion exchange.