The Kinetic and Spin-Orbit Densities in Kohn-Sham DFT

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Objective

- **Long Term Goal:**
  Calculation of bulk properties of the nuclei in a model-independent systematic way.

- **How to Generalize Skyrme HF?**
  For $N = Z$ nuclei, energy density $\mathcal{E}_{SK}(x)$ is:

  $$
  \mathcal{E}_{SK}(x) = \frac{1}{2M} \tau + \frac{3}{8} t_0 \rho^2 + \frac{1}{16} t_3 \rho^{2+\alpha}
  + \frac{1}{16} (3t_1 + 5t_2) \rho \tau + \frac{1}{64} (9t_1 - 5t_2)(\nabla \rho)^2
  - \frac{3}{4} W_0 \rho \nabla \cdot \mathbf{J} + \frac{1}{32} (t_1 - t_2) \mathbf{J}^2
  $$

  Variational procedure wrt. $\varphi_\alpha(x)$ gives:

  $$
  \left(-\nabla \frac{1}{2M^*(x)} \nabla + U(x) + \cdots\right) \varphi_\alpha(x) = \varepsilon_\alpha \varphi_\alpha(x)
  $$

  $$
  \rho(x) = \sum_\alpha |\varphi_\alpha(x)|^2 \quad \tau(x) = \sum_\alpha |\nabla \varphi_\alpha(x)|^2
  $$

**Plan:** Treat Skyrme HF as DFT.

How to go beyond HF systematically?

$\Rightarrow$ DFT in an EFT framework
Need for a Systematic Framework

Figure 6: Predicted two-neutron separation energies for the even-even Sn isotopes using several microscopic models based on effective nucleon-nucleon interactions and obtained with phenomenological mass formulas (shown in the inset). While calculations agree well in the region where experimental data are available, they diverge for neutron-rich isotopes with N>82. It is seen that the position of the neutron drip line is uncertain. Unknown nuclear deformations or as yet uncharacterized phenomena, such as the presence of neutron halos or neutron skins, make theoretical predictions highly uncertain. Experiments for the Sn isotopes with N=80–100 will greatly narrow the choice of viable models.
**DFT/EFT**

- **Kohn-Sham DFT:**
  
  \[ E[\rho(x)] = F_{HK}[\rho(x)] + \int d^3x \, v(x) \rho(x) \]

  \[ F_{HK}[\rho] = T_s[\rho] + E_{int}[\rho] \]

  Variational procedure wrt. \( \rho(x) \) gives:

  \[
  \left( -\frac{\nabla^2}{2M} + v_s(x) \right) \varphi_\alpha(x) = \varepsilon_\alpha \varphi_\alpha(x)
  \]

  \[ v_s(x) = v(x) + \frac{\delta E_{int}[\rho]}{\delta \rho(x)} \]

  **Key:** Exact \( \rho(x) = \sum_\alpha |\varphi_\alpha(x)|^2 \).

- **DFT/EFT calculates \( v_s(x) \) systematically:**

  \[
  \text{LO: } + \quad \text{NLO: } + \quad \text{NNLO: } +
  \]

  \[
  \text{LO: } + \quad \text{NLO: } + \quad \text{NNLO: } +
  \]
**EFT Lagrangian**

- **The first few terms**

\[
\mathcal{L}_{\text{EFT}} = \psi^\dagger \left[ i \partial_t + \mu + \frac{\nabla^2}{2M} \right] \psi - \frac{C_0}{2} (\psi^\dagger \psi)^2 \\
+ \frac{C_2}{16} \left[ (\psi \psi)^\dagger (\psi \nabla^2 \psi) + \text{hc.} \right] + \frac{C'_2}{8} (\psi \nabla \psi)^\dagger \cdot (\psi \nabla \psi)
\]

The coefficients are given in terms of effective-range parameters by:

\[
C_0 = \frac{4\pi a_s}{M}, \quad C_2 = C_0 \frac{a_s r_s}{2}, \quad \text{and} \quad C'_2 = \frac{4\pi a_p^3}{M}.
\]

- **Results for**

\[
E'_{C_2} [\rho] = \frac{(\nu - 1)}{4\nu} C_2 \int d^3x \frac{3}{5} \left( \frac{6\pi^2}{\nu} \right)^{2/3} (\rho^{8/3})
\]

\[
E_{C_2} [\rho, \tau] = \frac{(\nu - 1)}{4\nu} C_2 \int d^3x \left[ \rho \tau + \frac{3}{4} (\nabla \rho)^2 \right]
\]

The energy at NNLO has \(\tau\) dependence ... How can we incorporate this in the effective action formalism?
Effective Action Formalism

**Generating Functional**

\[
Z[J, \eta] = e^{iW[J, \eta]} = \int D\psi D\psi^\dagger e^{i \int d^4x \left[ \mathcal{L} + J(x)\psi^\dagger\psi + \eta(x)\nabla\psi^\dagger \cdot \nabla\psi \right]}
\]

The effective action is given by:

\[
\Gamma[\rho, \tau] = W[J, \eta] - \int d^4x \ J(x)\rho(x) - \int d^4x \ \eta(x)\tau(x)
\]

\[
\rho(x) \equiv \langle \psi^\dagger(x)\psi(x) \rangle_{J, \eta} = \frac{\delta W[J, \eta]}{\delta J(x)}
\]

\[
\tau(x) \equiv \langle \nabla\psi^\dagger(x) \cdot \nabla\psi(x) \rangle_{J, \eta} = \frac{\delta W[J, \eta]}{\delta \eta(x)}
\]

**Variational Procedure gives**:

\[
\left(-\nabla \frac{1}{2M^*(x)} \nabla + v_s(x)\right) \varphi_\alpha(x) = \varepsilon_\alpha \varphi_\alpha(x)
\]

\[
\frac{1}{2M^*(x)} = \frac{1}{2M} + \frac{\delta}{\delta \tau(x)}(E_{HF}[\rho] + E_c[\rho, \tau])
\]

\[
= \frac{1}{2M} + \left[ \frac{(\nu - 1)}{4\nu} C_2 + \frac{(\nu + 1)}{4\nu} C_2' \right] \rho(x)
\]

Looks like the Skyrme equation (for \( \nu = 4 \))!!
So does the energy density.


**Density for Hard-Sphere interaction**

\[(a_p = a_s, \ r_s = 2a_s/3)\]

\[
\begin{array}{c}
\begin{array}{c}
\text{Non-interacting} \\
\text{Kohn-Sham (KS) LO} \\
\text{KS NLO} \\
\text{KS NNLO} \\
\text{Hard Sphere} \\
\text{\(A = 240, a_s = 0.16, \nu = 2\)}
\end{array}
\end{array}
\]

**Energy Estimates**

\[
\begin{array}{c}
\begin{array}{c}
\nu = 4, a_s = 0.10, A = 140
\end{array}
\end{array}
\]

\[
\begin{array}{c}
\begin{array}{c}
\text{LO} \\
\text{NLO} \\
\text{LDA} \\
\text{\(\rho\)} \\
\text{\(10^* (\nabla \rho)\)} \\
\text{\(\tau\) - NNLO}
\end{array}
\end{array}
\]

\[
\begin{array}{c}
\begin{array}{c}
\text{\(a_p = a_s\)} \\
\text{\(a_p = 0\)}
\end{array}
\end{array}
\]
**Effective Mass**

$M^*/M = 0.93$

$n = 1$

$a_p = a_s$

$n = 4$

$n = 3$

$n = 2$

$n = 1$

$r/t \tau = 0$

$l = 0$

$l = 7$

$a_s = 0.16$, $r_s = 2a_s/3$

$v = 2$, $N_F = 7$, $A = 240$

**Compare Energy Spectra for $\rho$ and $\rho\tau$-DFT**

$M^*(0)/M = 0.73$

$n = 4$

$n = 3$

$n = 2$

$n = 1$

$r/t \tau = 0$

$l = 0$

$l = 7$
Comparison to Actual Spectra

- Introduce a non-local source $\xi(x, x')$
coupled to $\psi(x)\psi^\dagger(x')$:

$$Z[J, \eta] \rightarrow Z[J, \eta, \xi]$$

Compute the effective action:

$$\Gamma[\rho, \tau] \rightarrow \Gamma[\rho, \tau, \xi]$$

- Construct the full Green’s Function:

$$G = G_{\text{ks}} + \Sigma'_{\text{ks}} + G_{\text{ks}}$$

- Densities agree by construction...

$$x \bigcirc = x \bigcirc + x \bigcirc \bigcirc + x \bigcirc \bigcirc \bigcirc = x \bigcirc$$

- But Single-Particle Spectra differ:

$$\varepsilon_\rho^k - \varepsilon_{\rho\tau}^k = \left[ \frac{\nu - 1}{4\nu} C_2 + \frac{\nu + 1}{4\nu} C'_2 \right] \rho (k_F^2 - k^2)$$
Incorporating Spin-Orbit

- **Spin-Orbit Lagrangian**

\[ \mathcal{L}_{SO} = -i \frac{C_2^g}{4} \sigma \cdot (\psi \nabla \psi)^\dagger \times (\psi \nabla \psi) \]

The expanded version looks like:

\[
(\psi^\dagger \nabla \psi) \cdot (\nabla \psi^\dagger \times \sigma \psi) + (\nabla \psi^\dagger \psi) \cdot (\psi^\dagger \sigma \times \nabla \psi) \\
-(\psi^\dagger \psi)(\nabla \psi^\dagger \cdot \sigma \times \nabla \psi) + (\psi^\dagger \sigma \psi) \cdot (\nabla \psi^\dagger \times \nabla \psi)
\]

- **Contribution to Energy:**

\[
E_{C_2}[\rho, \tau, J] = -\frac{C_2^g}{2} \left( 1 + \frac{1}{\nu_{iso}} \right) \int d^3x \rho \nabla \cdot J(x)
\]

\[
iJ(x) = \nu_{iso} \sum_k \psi_k^\dagger(x)(\nabla \times \sigma_{\alpha \beta})\psi_{k\beta}(x)
\]

How to incorporate \( J \) in the Effective Action Formalism?
Incorporating $J$

- **Introduce a vector source** $\xi(x)$ coupled to $J(x)$ (spin-orbit density):

$$Z[J, \eta] \to Z[J, \eta, \xi]$$

The effective action is given by:

$$\Gamma[\rho, \tau, \xi] = W[J, \eta, \xi] - \int d^4x \ J(x) \rho(x)$$

$$- \int d^4x \ \eta(x) \tau(x) - \int d^4x \ \xi(x) \cdot J(x)$$

$$\rho(x) \equiv \langle \psi^\dagger(x) \psi(x) \rangle_J, \eta, \xi = \frac{\delta W[J, \eta, \xi]}{\delta J(x)}$$

$$\tau(x) \equiv \langle \nabla \psi^\dagger(x) \cdot \nabla \psi(x) \rangle_J, \eta, \xi = \frac{\delta W[J, \eta, \xi]}{\delta \eta(x)}$$

$$J(x) \equiv -i \langle \psi^\dagger(x) (\nabla \times \sigma) \psi(x) \rangle_J, \eta, \xi = \frac{\delta W[J, \eta, \xi]}{\delta \xi(x)}$$

- **Variational Procedure gives**:

$$\widehat{H} \varphi_\alpha(x) = \varepsilon_\alpha \varphi_\alpha(x)$$

$$\widehat{H} = \left( -\nabla \cdot \frac{1}{2M^*(x)} \nabla + v_s(x) + i \xi_0 \cdot \nabla \times \sigma \right)$$

$$\xi_0(x) = -\frac{\delta}{\delta J(x)} (E_{\text{int}}[\rho, \tau, J])$$

$$= \left( \frac{\nu_{\text{iso}} + 1}{2 \nu_{\text{iso}}} \right) C_2 \nabla \rho(x)$$
Estimating the Spin-Orbit Contribution

\[ v = 4, a_s = 0.10, A = 140 \]
Summary

- Kinetic energy density $\tau$ was incorporated in EFT/DFT through an effective action formalism. Single-particle Kohn-Sham Eq. with $M^*(x)$ was solved in a harmonic trap.

- Ground state energy density found to be of the Skyrme form, with $\rho\tau$, $\nabla\rho$ and $\rho^{2+\alpha}$ pieces.

- Energy spectra are different for $\rho$ and $\rho\tau$ case even though the total energy and density are almost the same. The $\rho\tau$ spectra is closer to the actual spectra.

- Spin-Orbit density $J$ was incorporated in EFT/DFT.
Work in Progress

- Gradient corrections to $\bullet$ + $\cdots$
- Include all terms up to two derivatives in spin-dependent potential
- Include isospin dependence and tensor piece potential
- Generalize to include pairing
- Include long range forces in the framework to establish a connection to chiral effective field theories with pions
- Investigate connection of effective low-momentum potential approach to DFT approach
- Incorporate time dependence to study collective modes
- Address issues relating to self-bound systems