The Kinetic Energy Density in Kohn-Sham Density Functional Theory

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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 $\mathcal{E}_{SK}(\mathbf{x})$ is:

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

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

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

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

Plan: Treat Skyrme HF as DFT.

How to go beyond HF systematically?

⇒ DFT in an EFT framework

DFT/EFT

- **Kohn-Sham DFT:**

$$E[\rho(\mathbf{x})] = F_{HK}[\rho(\mathbf{x})] + \int d^3\mathbf{x}\, v(\mathbf{x})\rho(\mathbf{x})$$

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

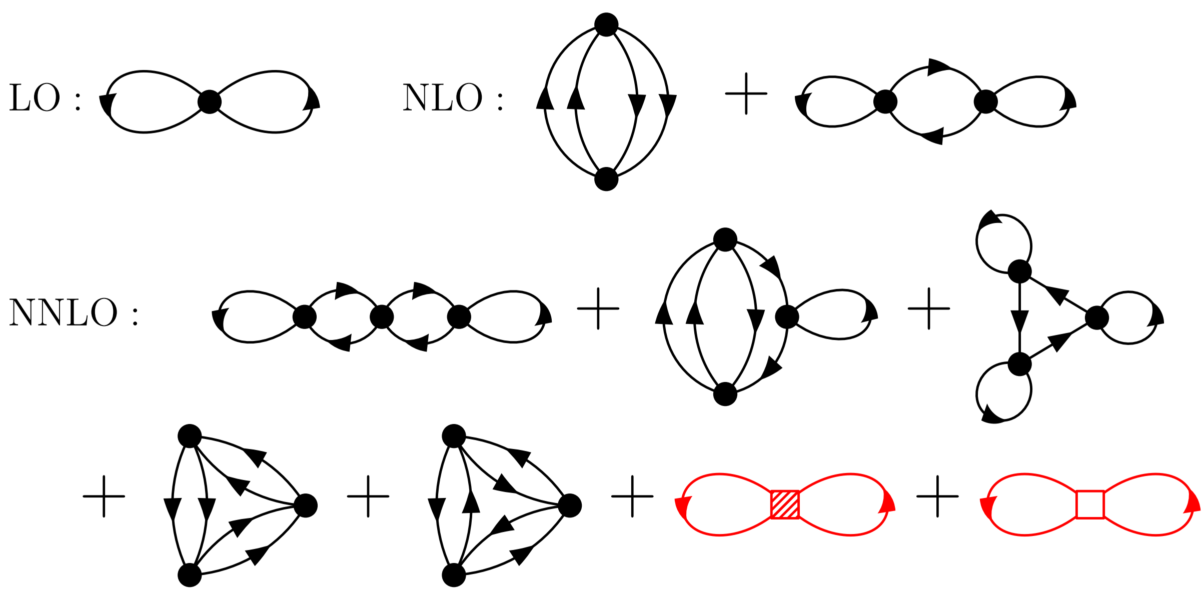
Variational procedure wrt. $\rho(\mathbf{x})$ gives :

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

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

Key : Exact $\rho(\mathbf{x}) = \sum_\alpha |\varphi_\alpha(\mathbf{x})|^2$.

- **DFT/EFT calculates $v_s(\mathbf{x})$ systematically:**



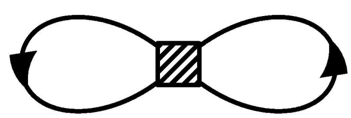
EFT Lagrangian

- **The first few terms**

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

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** 

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

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

The energy at NNLO has τ dependence ... How can we incorporate this in the effective action formalism?

Effective Action Formalism

- **Generating Functional**

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

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 :**

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

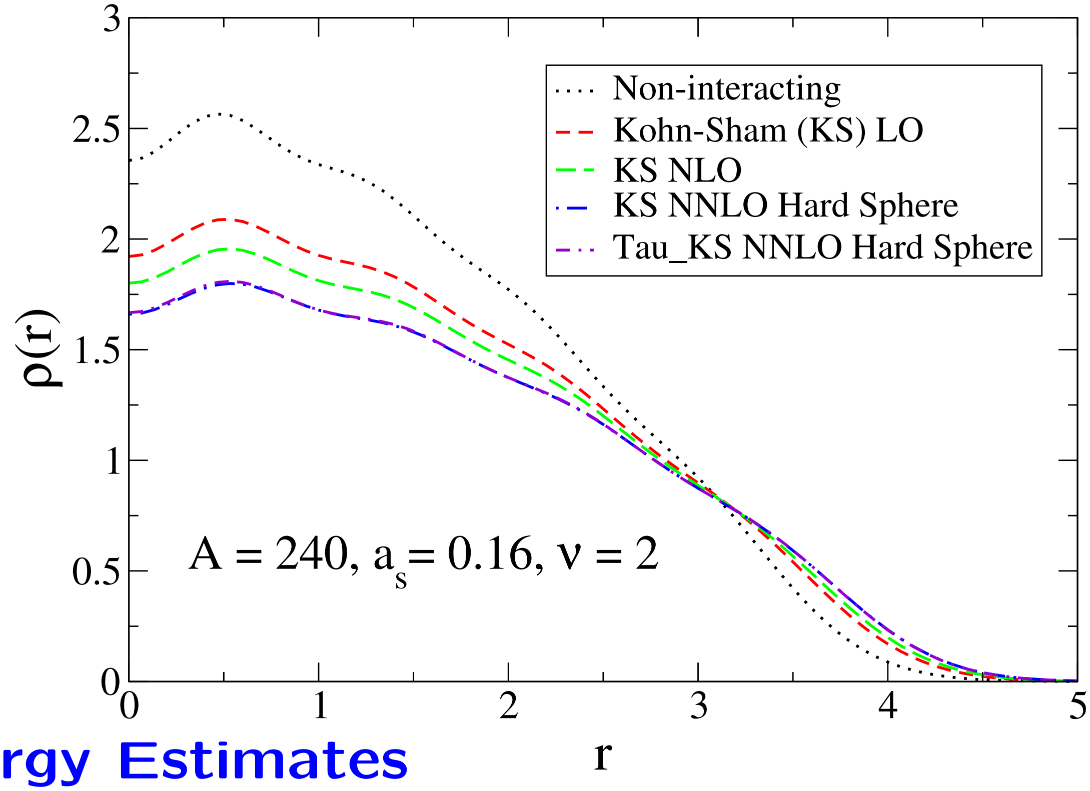
$$\frac{1}{2M^*(\mathbf{x})} = \frac{1}{2M} + \frac{\delta}{\delta\tau(\mathbf{x})}\left(E_{\mathrm{HF}}[\rho] + E_c[\rho,\tau]\right)$$
$$= \frac{1}{2M} + \left[\frac{(\nu-1)}{4\nu}C_2 + \frac{(\nu+1)}{4\nu}C_2'\right]\rho(\mathbf{x})$$

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

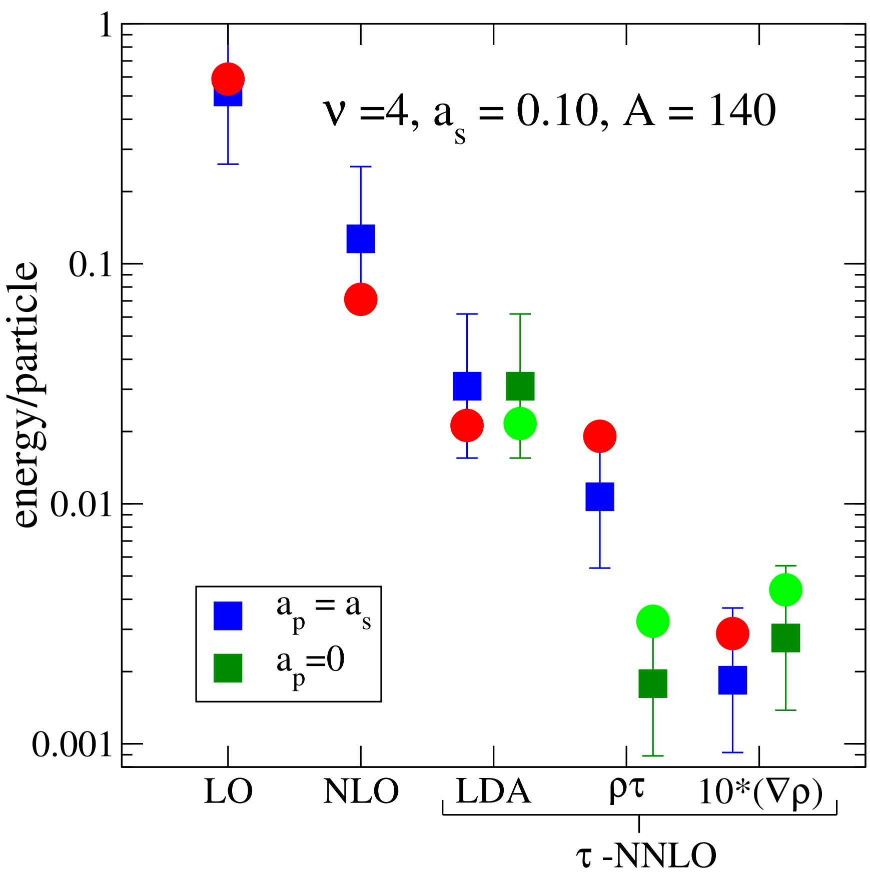
Results

- **Density for Hard-Sphere interaction**

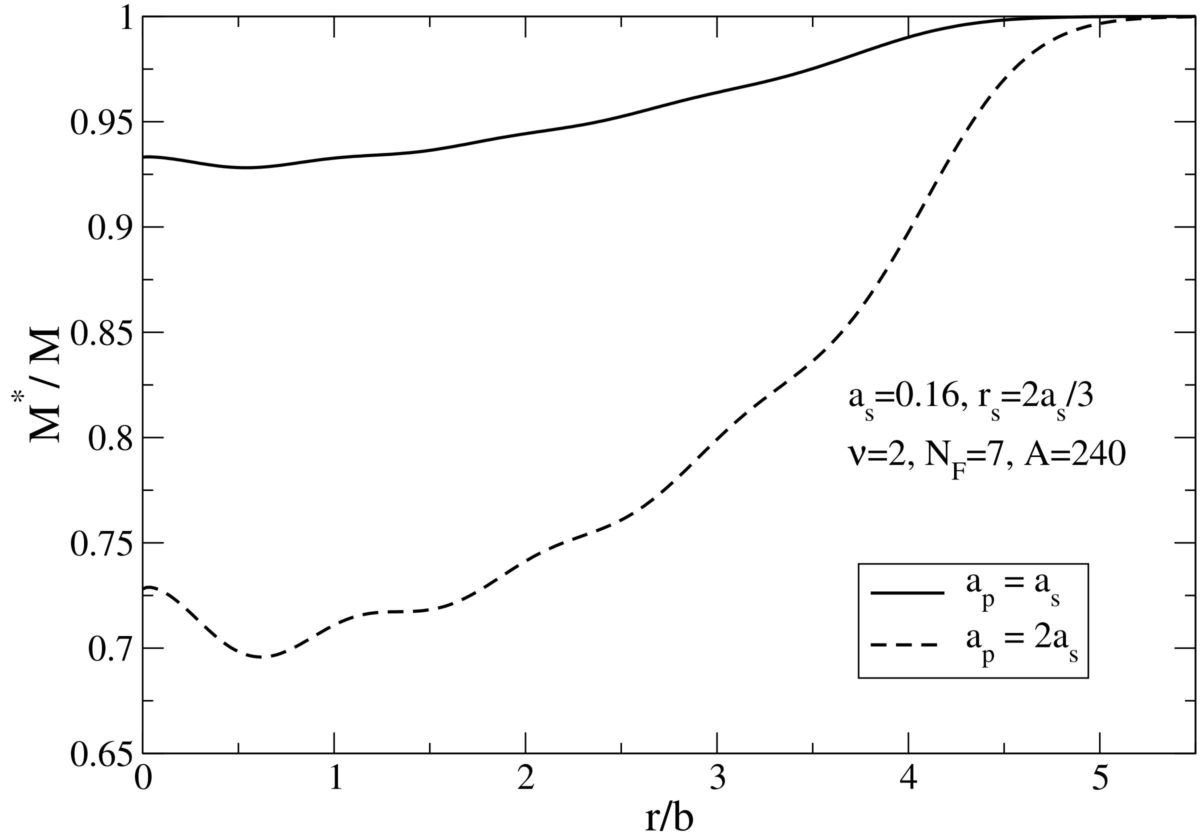
$$(a_p = a_s,\ \ r_s = 2a_s/3)$$



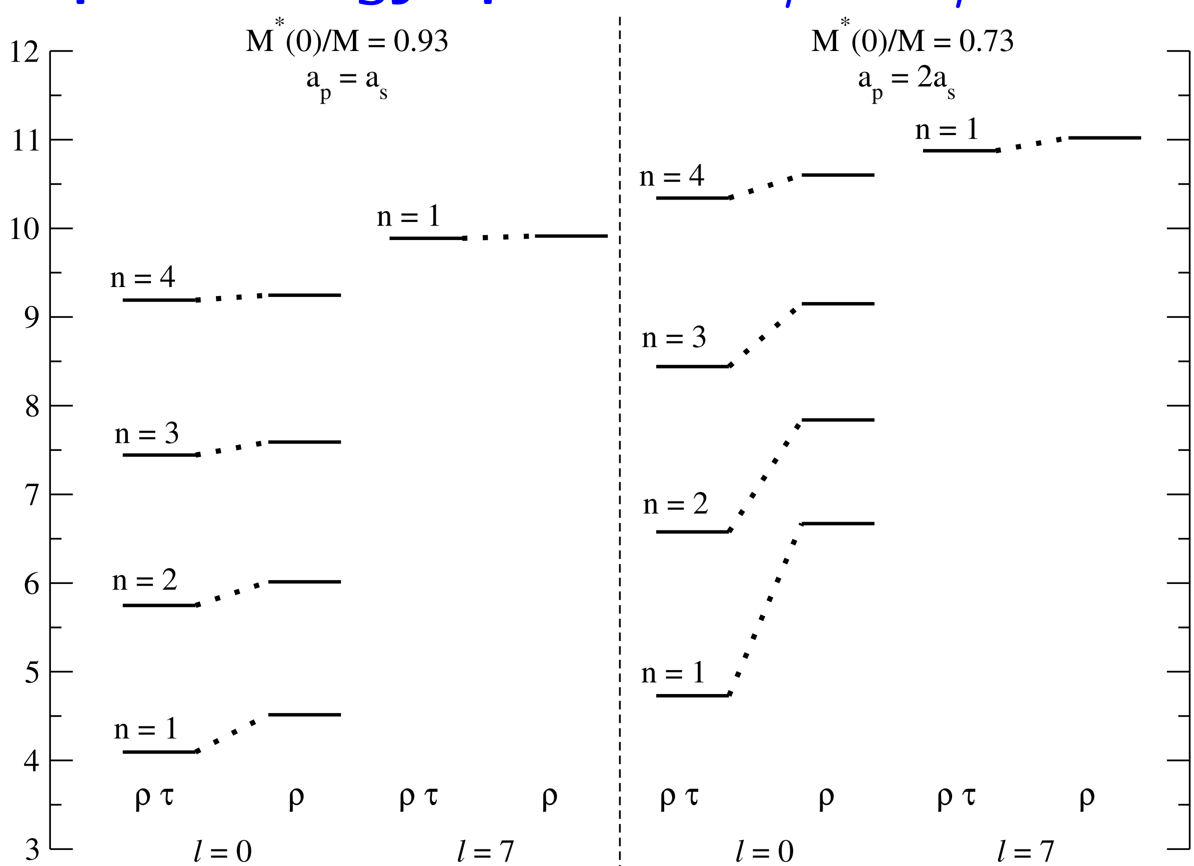
- **Energy Estimates**



- **Effective Mass**



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



Comparison to Actual Spectra

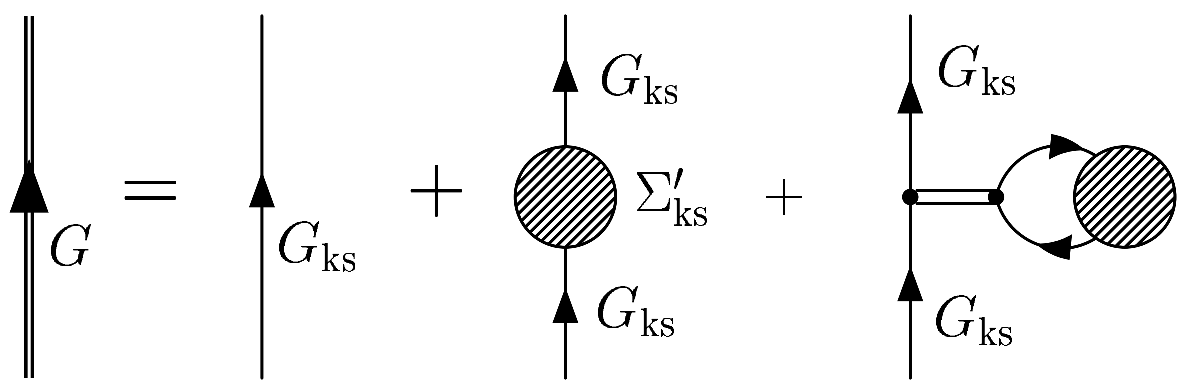
- **Introduce a non-local source $\xi(x,x')$ coupled to $\psi(x)\psi^\dagger(x')$:**

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

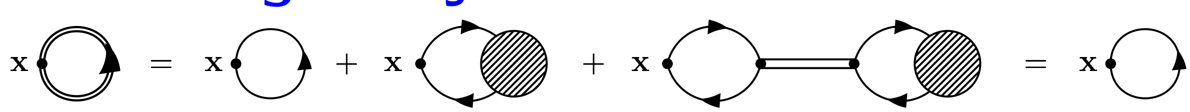
Compute the effective action :

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

- **Contruct the full Green's Function :**



- **Densities agree by construction...**



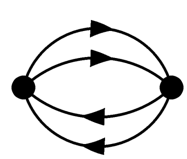
- **But Single-Particle Spectra differ :**

$$\varepsilon_k^{\rho} - \varepsilon_k^{\rho\tau} = \left[\frac{(\nu-1)}{4\nu}\,C_2 + \frac{(\nu+1)}{4\nu}\,C_2^{'}\right]\rho\,(k_F^2 - k^2)$$

Summary

- Kinetic energy density τ was incorporated in EFT/DFT through an effective action formalism. Single-particle Kohn-Sham Eq. with $M^*(\mathbf{x})$ 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 ρ 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.

Future Plans

- Gradient corrections to  $+ \cdots$
- Add spin-orbit interactions
- Generalize to include pairing