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

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

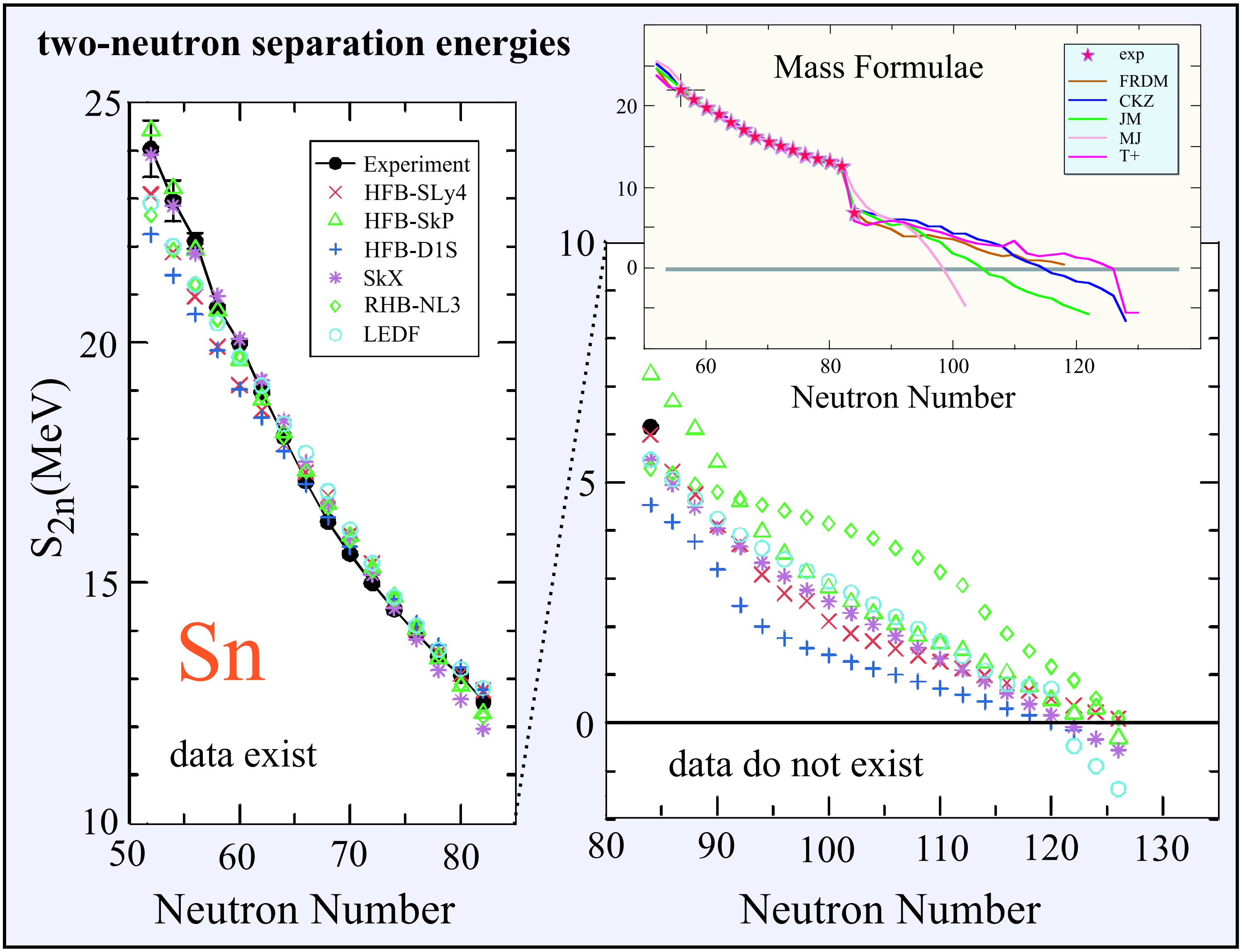
$$\rho(\mathbf{x}) = \sum_\alpha |\varphi_\alpha(\mathbf{x})|^2 \quad \tau(\mathbf{x}) = \sum_\alpha |\nabla\varphi_\alpha(\mathbf{x})|^2$$

Plan: Treat Skyrme HF as DFT.

How to go beyond HF systematically?

$\Rightarrow$ DFT in an EFT framework

Need for a Systematic Framework



DFT/EFT

- **Kohn-Sham DFT:**

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

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

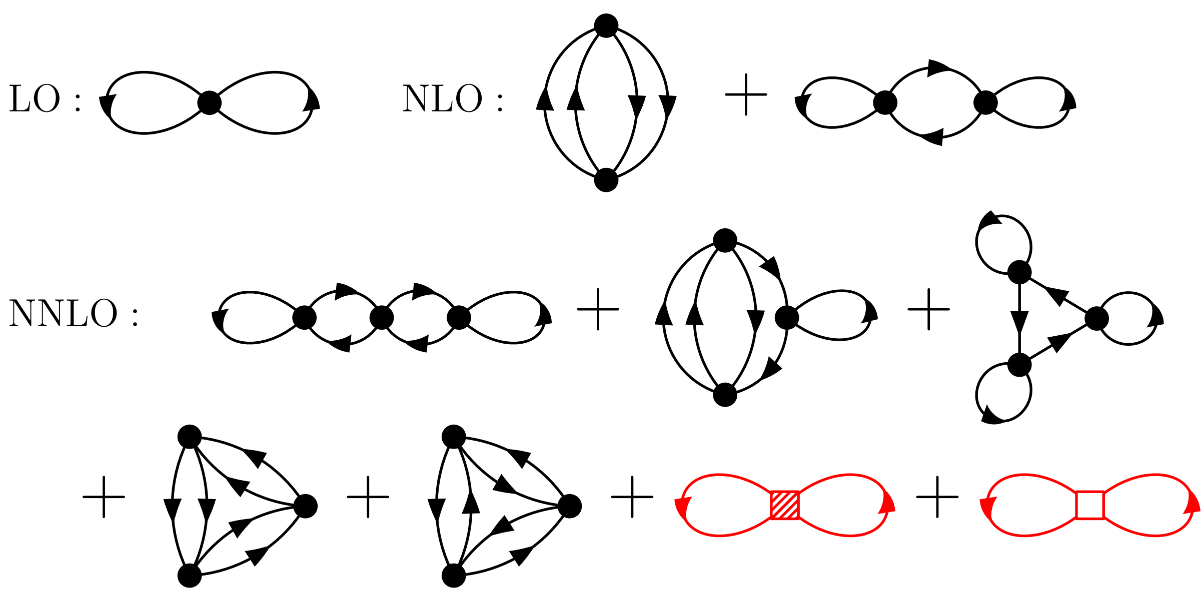
Variational procedure wrt. $\rho(\mathbf{x})$ gives :

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

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

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

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



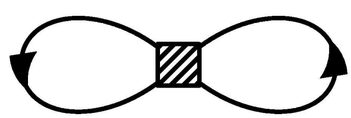
EFT Lagrangian

- **The first few terms**

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

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**

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

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 :**

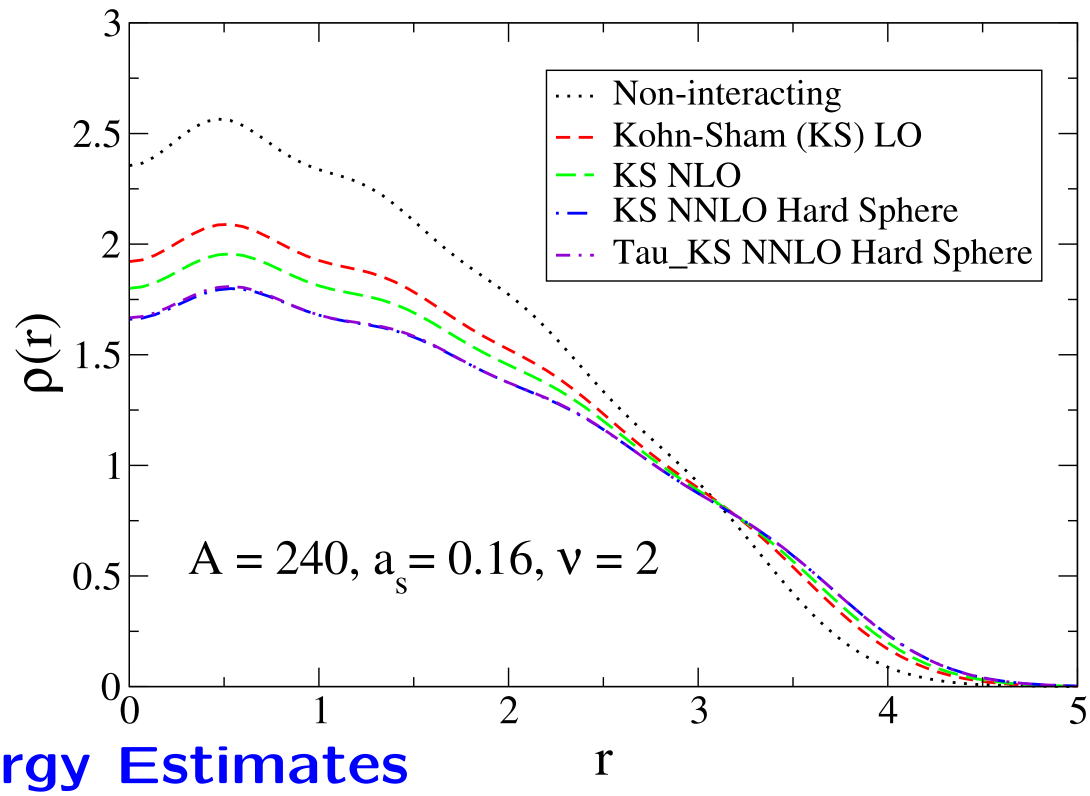
$$
\left(-\nabla\frac{1}{2M^*(\mathbf{x})}\nabla + v_s(\mathbf{x})\right)\varphi_\alpha(\mathbf{x}) = \varepsilon_\alpha\varphi_\alpha(\mathbf{x})
$$

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

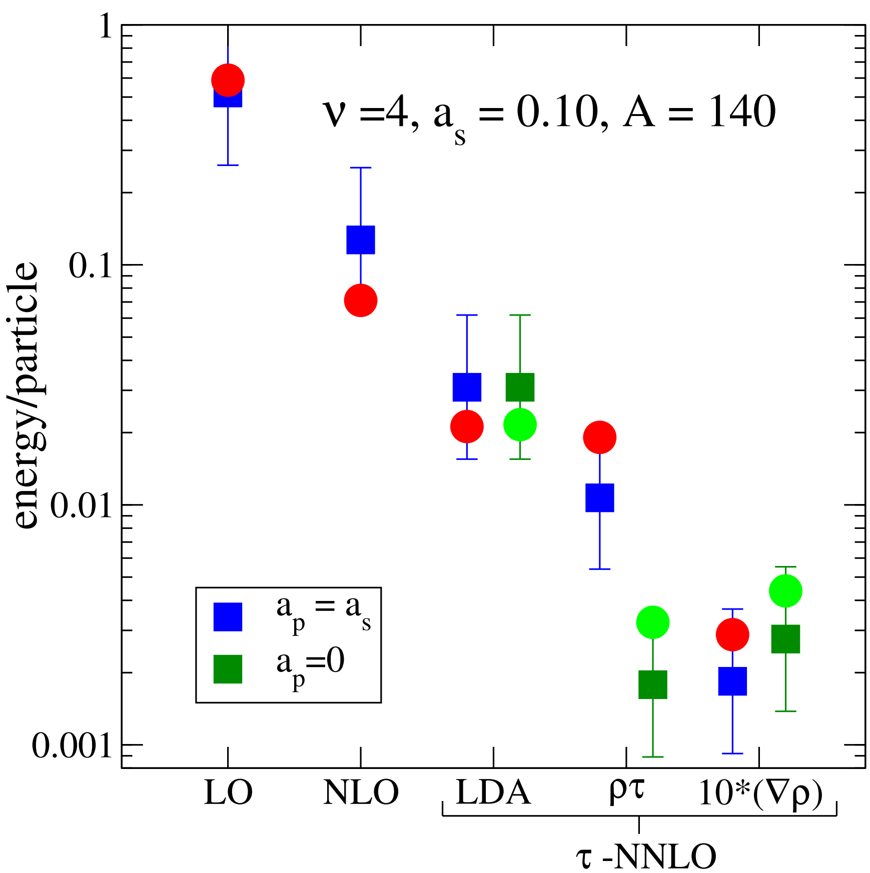
Looks like the Skyrme equation (for $\nu = 4$)!!
So does the energy density.

- **Density for Hard-Sphere interaction**

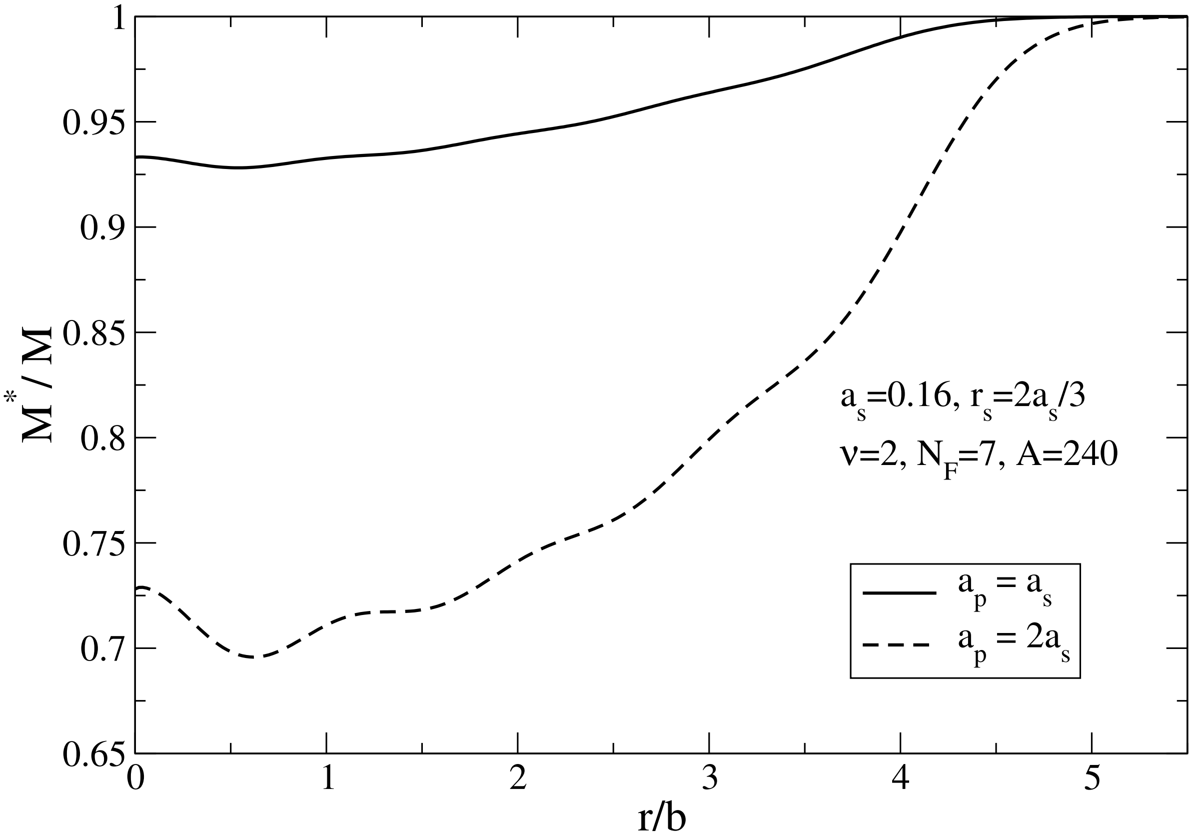
$$(a_p = a_s,\ r_s = 2a_s/3)$$



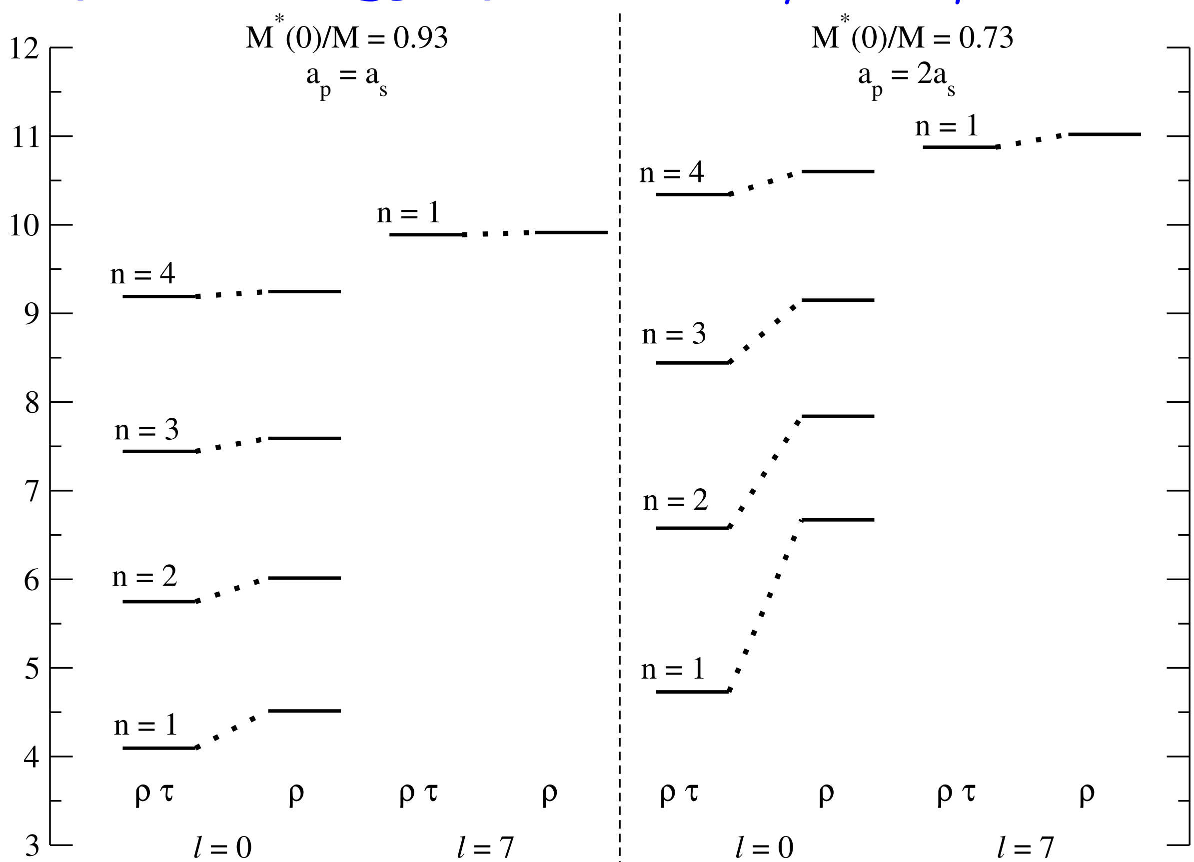
- **Energy Estimates**



- **Effective Mass**



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



Comparison to Actual Spectra

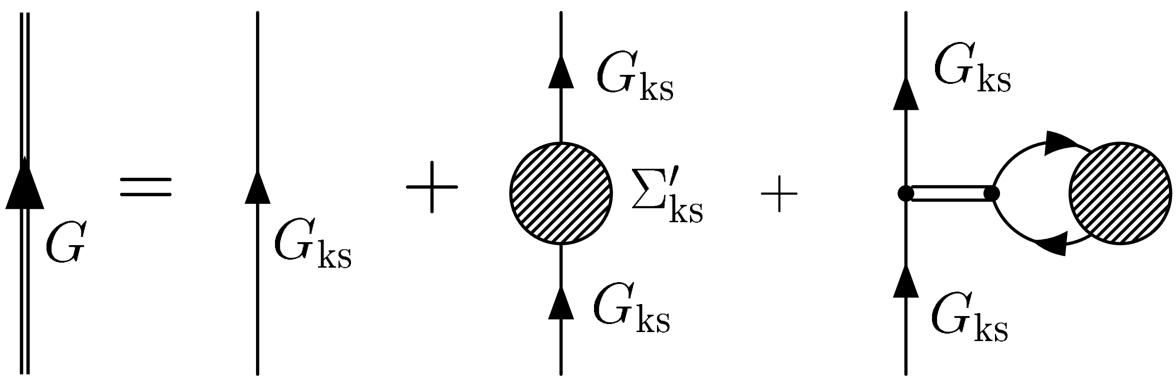
- **Introduce a non-local source $\xi(x, x')$ coupled to $\psi(x)\psi^\dagger(x')$:**

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

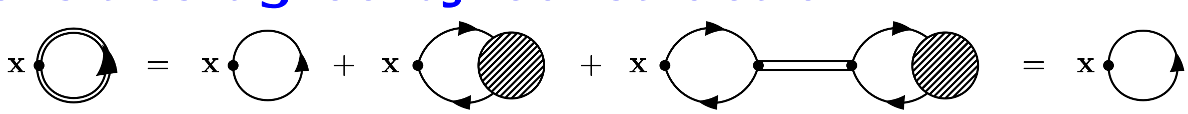
Compute the effective action :

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

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



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



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

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

Incorporating Spin-Orbit

- **Spin-Orbit Lagrangian**

$$\mathcal{L}_{\mathsf{SO}} = -i\frac{C_2^\sigma}{4}\boldsymbol{\sigma}\cdot(\psi\overleftrightarrow{\boldsymbol{\nabla}}\psi)^\dagger\times(\psi\overleftrightarrow{\boldsymbol{\nabla}}\psi)$$

The expanded version looks like :

$$(\psi^\dagger\boldsymbol{\nabla}\psi)\cdot(\boldsymbol{\nabla}\psi^\dagger\times\boldsymbol{\sigma}\psi)+(\boldsymbol{\nabla}\psi^\dagger\psi)\cdot(\psi^\dagger\boldsymbol{\sigma}\times\boldsymbol{\nabla}\psi)$$
$$-(\psi^\dagger\psi)(\boldsymbol{\nabla}\psi^\dagger\cdot\boldsymbol{\sigma}\times\boldsymbol{\nabla}\psi)+(\psi^\dagger\boldsymbol{\sigma}\psi)\cdot(\boldsymbol{\nabla}\psi^\dagger\times\boldsymbol{\nabla}\psi)$$

- **Contribution to Energy:**

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

$$i\boldsymbol{J}(\mathbf{x}) = \nu_{\mathsf{iso}}\sum_k\psi^\dagger_{k\alpha}(\mathbf{x})(\boldsymbol{\nabla}\times\boldsymbol{\sigma}_{\alpha\beta})\psi_{k\beta}(\mathbf{x})$$

How to incorporate $\boldsymbol{J}$ in the Effective Action Formalism?

Incorporating J

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

$$Z[J,\eta] \to Z[J,\eta,\boldsymbol{\xi}]$$

The effective action is given by :

$$\begin{aligned}\Gamma[\rho,\tau,\boldsymbol{\xi}] &= W[J,\eta,\boldsymbol{\xi}] - \int d^4x\, J(x)\rho(x) \\ &\quad - \int d^4x\, \eta(x)\tau(x) - \int d^4x\, \boldsymbol{\xi}(x)\cdot \boldsymbol{J}(x)\end{aligned}$$

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

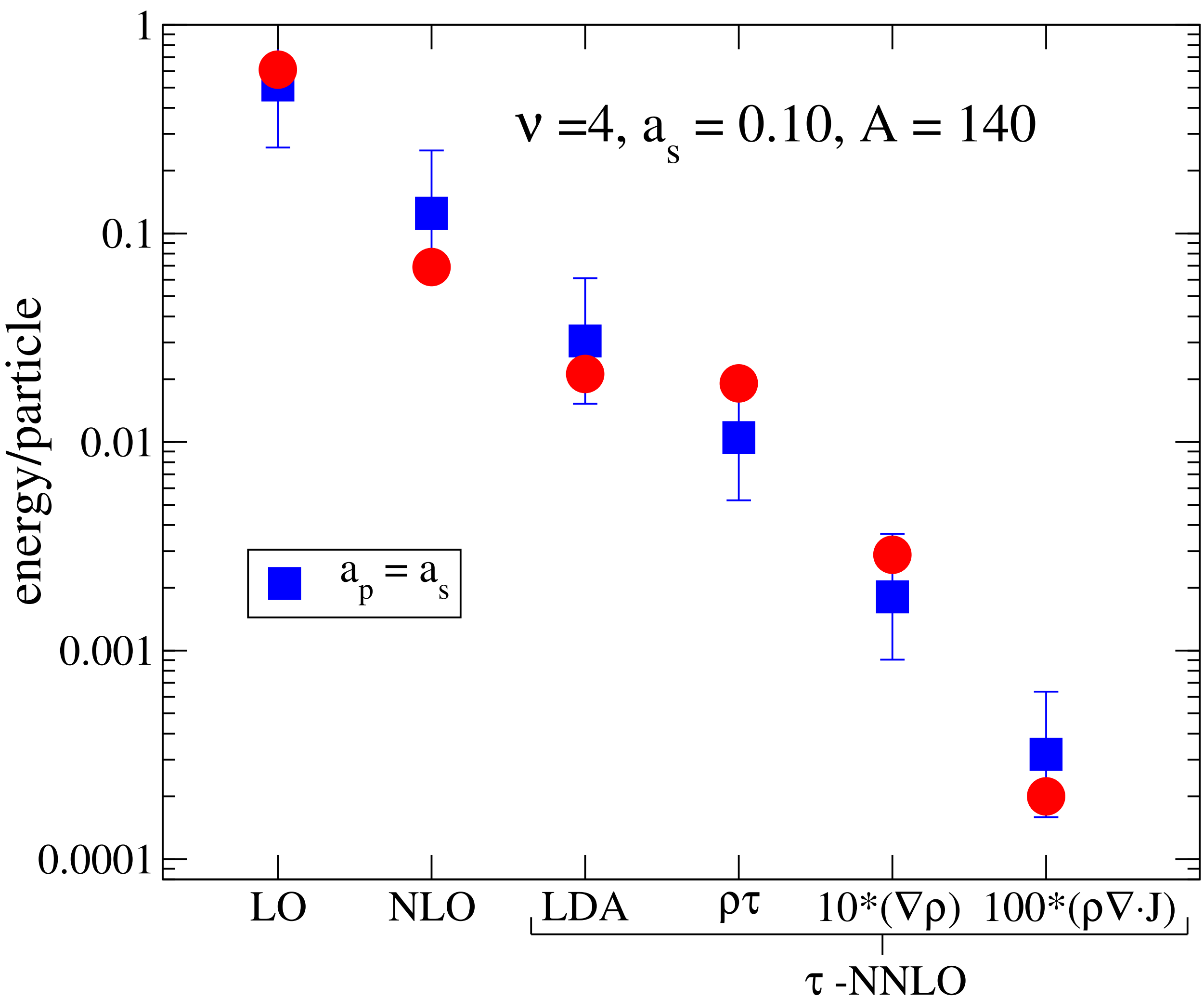
$$\tau(x) \equiv \langle \nabla\psi^\dagger(x)\cdot\nabla\psi(x)\rangle_{J,\eta,\boldsymbol{\xi}} = \frac{\delta W[J,\eta,\boldsymbol{\xi}]}{\delta \eta(x)}$$

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

- **Variational Procedure gives :**

$$\begin{aligned}\widehat{H}\,\varphi_\alpha(\mathbf{x}) &= \varepsilon_\alpha\varphi_\alpha(\mathbf{x}) \\ \widehat{H} &= \left(-\nabla\cdot\frac{1}{2M^*(\mathbf{x})}\nabla + v_s(\mathbf{x}) + i\boldsymbol{\xi}_0\cdot\boldsymbol{\nabla}\times\boldsymbol{\sigma}\right) \\ \boldsymbol{\xi}_0(\mathbf{x}) &= -\frac{\delta}{\delta\boldsymbol{J}(\mathbf{x})}\left(E_{\text{int}}[\rho,\tau,\boldsymbol{J}]\right) \\ &= -\left(\frac{\nu_{\text{iso}}+1}{2\nu_{\text{iso}}}\right) C_2^\sigma\,\boldsymbol{\nabla}\rho(\mathbf{x})\end{aligned}$$

Estimating the Spin-Orbit Contribution



Summary

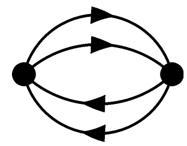
- Kinetic energy density τ was incorporated in EFT/DFT through an effective action formalism. Single-particle Kohn-Sham Eq. with $M^*(\mathbf{x})$ was solved in a harmonic trap.

- 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.

- Spin-Orbit density $\boldsymbol{J}$ was incorporated in EFT/DFT.

Work in Progress

- Gradient corrections to  $+\cdots$
- Include all terms upto 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