

# Functional Renormalization Group of the Nuclear Energy Density Functional Method

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# Outline

## 1 Context

*Where does the EDF method stand within the landscape of nuclear structure theories ?*

## 2 Lessons from empirical EDFs

*1<sup>st</sup> lesson : Effective (pseudo-)Hamiltonians with simple forms do the job*

*2<sup>nd</sup> lesson : Static correlations can be optimally grasped via SSBs + bosonic fluctuations of order parameters*

## 3 Towards a rigorous formulation of nuclear EDFs

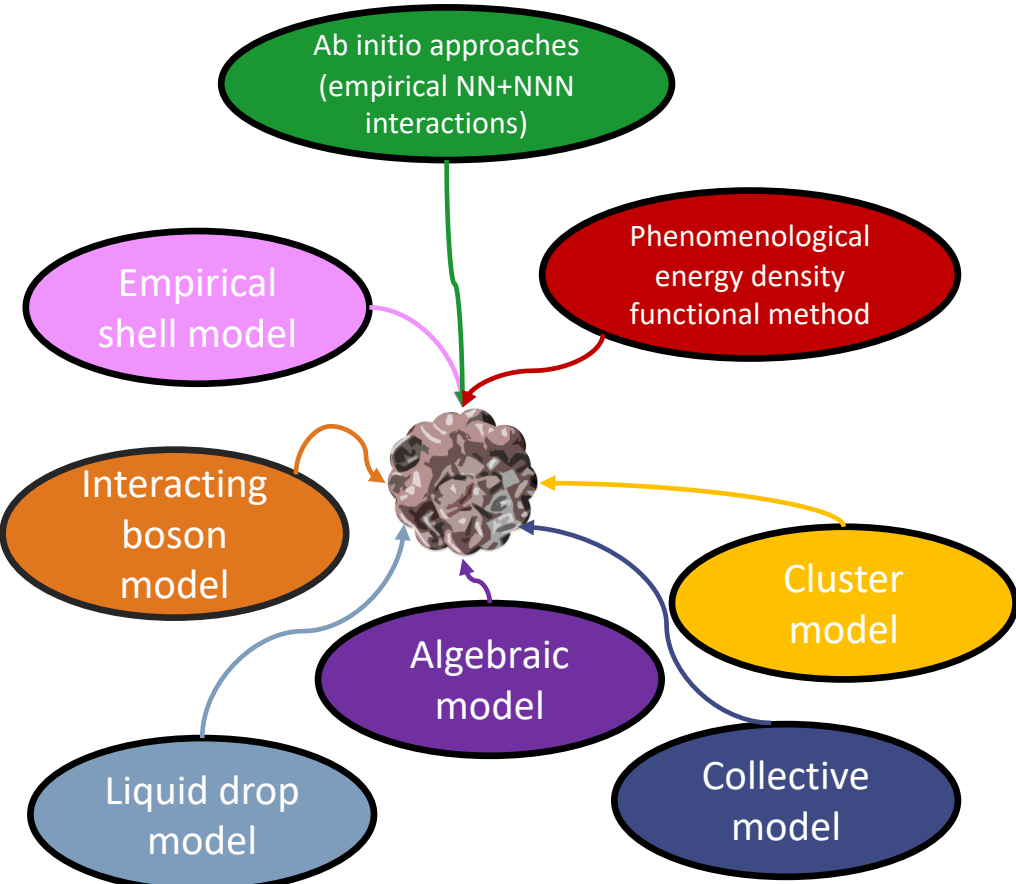
*WFT, DFT & EA perspectives*

*FRG*

*Application to symmetric nuclear matter*

# 1 Context : Strategies

## Era of models



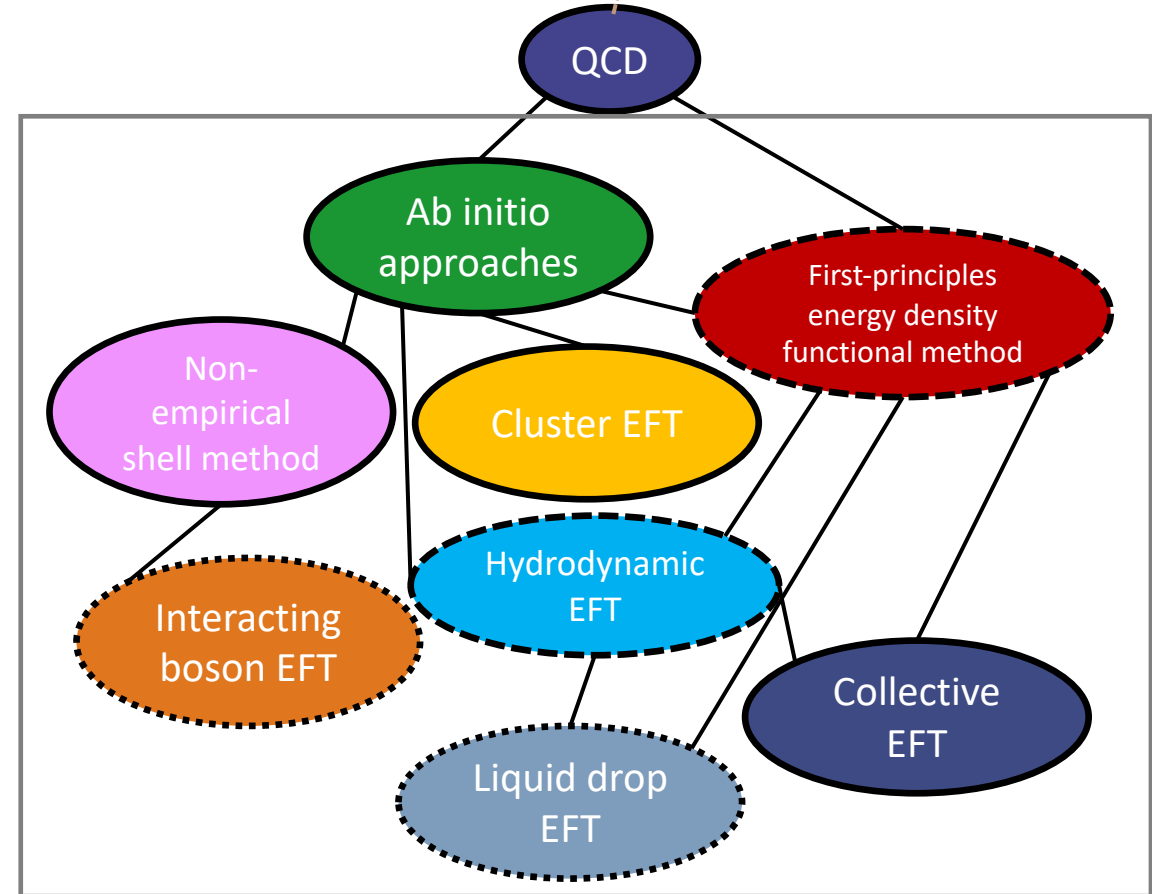
- ✓ Gives insight about relevant scales/dofs
- ✓ Ready to be used
- ✗ Lack of control  
⇒ double counting issues, error compensation, no error assessment

⊙ Achieve a

accurate  
predictive  
computationally affordable

description ?

## Era of effective (field) theories



- ✓ Full control ⇒ systematically improvable, no error compensation, no double counting, possibility of error estimation, ...
- ✓ ✗ Force you to step back and rethink

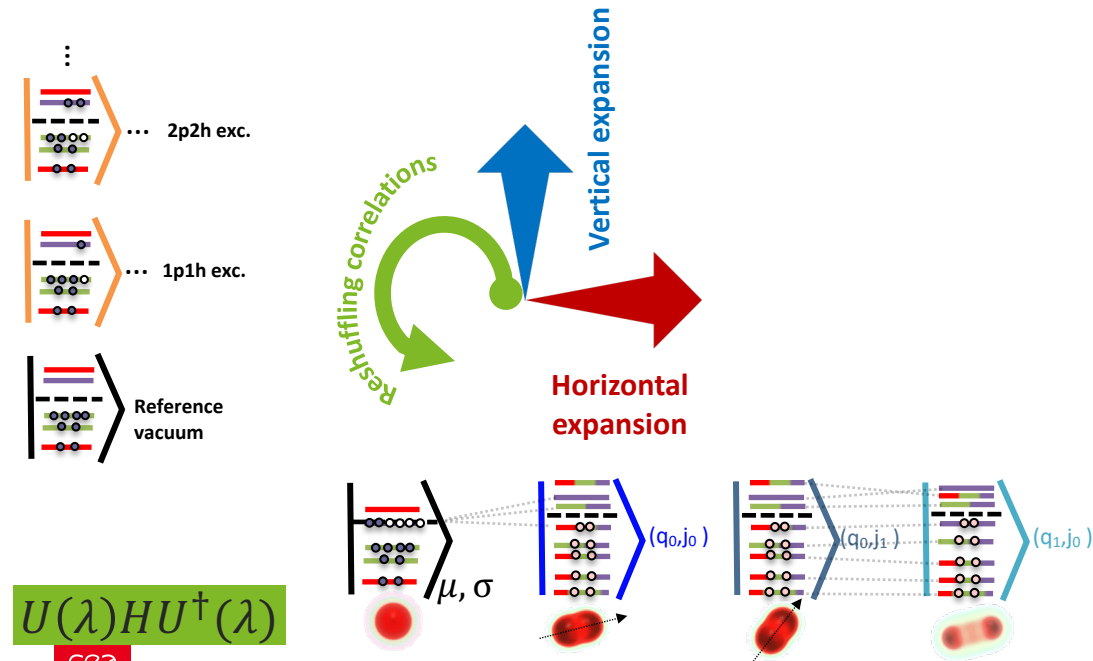
# 1 Context : Nuclear structure from a microscopic viewpoint

- 1) Nucleus:  $A$  interacting, structure-less nucleons
- 2) Structure & dynamic encoded in Hamiltonian, Functional, ...
- 3) Solve  $A$ -nucleon Schrödinger/Dirac equation to desired accuracy

$$H(\text{wavy nucleons}, \dots) |\Psi_{\mu, \sigma}\rangle = E_{\mu\sigma} |\Psi_{\mu, \sigma}\rangle$$

Strongly correlated WF

## Rationale for grasping nucleon correlations



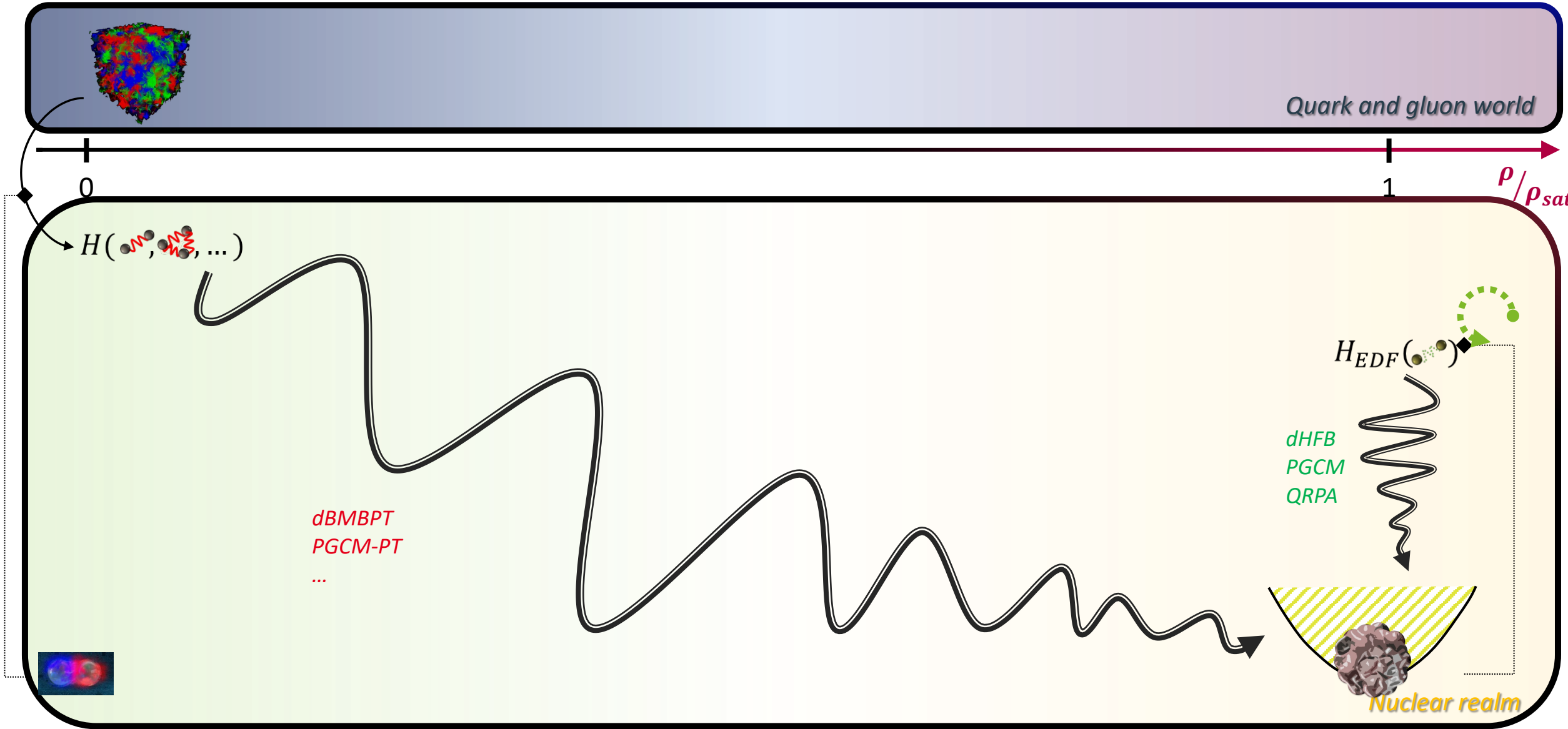
## Ab initio

- ⊙ Systematically improvable free-space Hamiltonian in  $\chi$ EFT
- ⊙ Solving Schrödinger equation
  - ◇ Pre-processing H
  - ◇ Refined many-body schemes with controlled uncertainties
    - CI (full space diag.) : exponential scaling
    - Hybrids (valence space diag.) : mixed scaling
    - Expansion methods (partition, expand and truncate) : polynomial scaling
- ⊗ How to challenge ab initio frontiers

## EDF

- ⊙ Effective pseudo-Hamiltonian
  - Free-space interactions  $\rightarrow$  Effective in-medium interactions
  - $|\Psi_{\mu, \sigma}\rangle$  Complicated WF  $\rightarrow$   $|\Theta_{\mu\sigma}\rangle$  Simplified auxiliary WF
- ⊙ Various levels of realization
  - Hartree-Fock-Bogoliubov (HFB)
  - Projected Generator Coordinate Method (PGCM)
  - Quasiparticle Random Phase Approximation (QRPA)
- ⊗ How to improve current EDFs
- ⊗ How to turn EDF in EFT?

# 1 Context : Nuclear structure from a microscopic viewpoint



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*WFT, DFT & EA perspectives*

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# 2 Lessons from empirical EDFs : main idea



Hamiltonian  $H$  acting in  $\mathcal{H}_A$  and Schrödinger equation

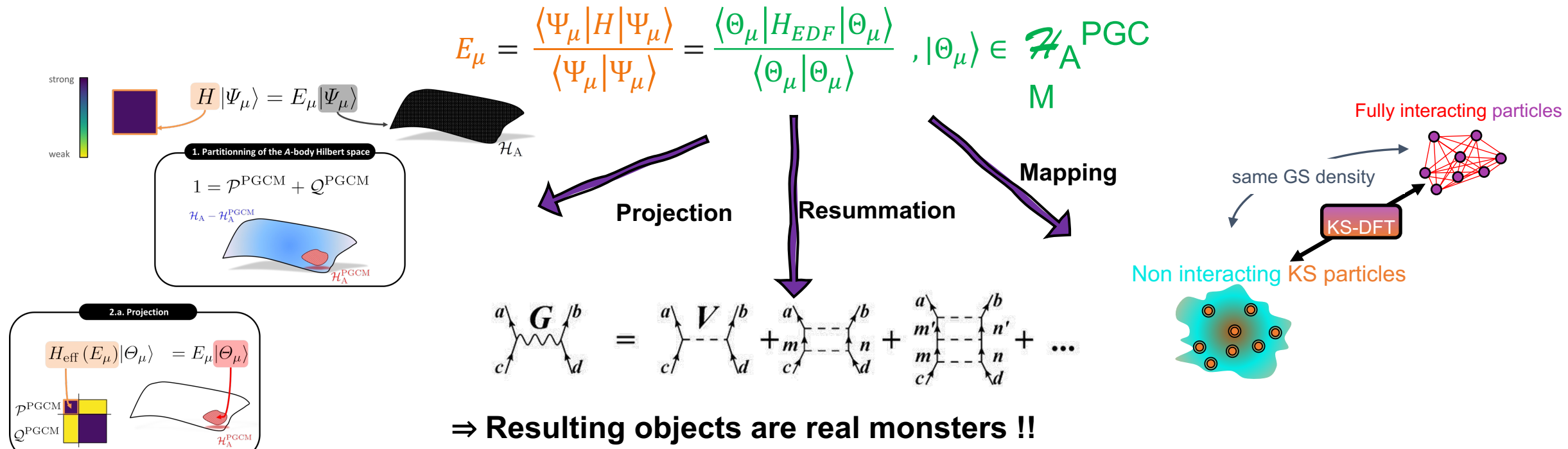
$$H = T + V + W + \dots$$

$$= \frac{1}{(1!)^2} \sum_{\substack{a_1 \\ b_1}} t_{b_1}^{a_1} A_{b_1}^{a_1} + \frac{1}{(2!)^2} \sum_{\substack{a_1 a_2 \\ b_1 b_2}} v_{b_1 b_2}^{a_1 a_2} A_{b_1 b_2}^{a_1 a_2} + \frac{1}{(3!)^2} \sum_{\substack{a_1 a_2 a_3 \\ b_1 b_2 b_3}} w_{b_1 b_2 b_3}^{a_1 a_2 a_3} A_{b_1 b_2 b_3}^{a_1 a_2 a_3} + \dots$$

$$A_{b_1 \dots b_k}^{a_1 \dots a_k} \equiv c_{a_1}^\dagger \dots c_{a_k}^\dagger c_{b_k} \dots c_{b_1}$$

$$H|\Psi_\mu\rangle = E_\mu|\Psi_\mu\rangle$$

EDF method postulates the existence of  $H_{EDF}$  acting in  $\mathcal{H}_A^{PGCM}$  yielding the same low-energy observables than with  $H$





# 2 Lessons from empirical EDFs : Lesson 1

● Empirical effective interactions with simple forms do the job !!

## Galilean EDF

## Lorentzian EDF

Explicit  
density-dependence

### Gogny D1 vertex

$$V_{12} = \sum_{i=1,2} (W_i + B_i P_\sigma - H_i P_\tau - M_i P_\sigma P_\tau) e^{-\frac{(\vec{r}_1 - \vec{r}_2)^2}{\mu_i^2}} \\ + t_0 (1 + x_0 P_\sigma) \delta(\vec{r}_1 - \vec{r}_2) \rho^\alpha \left( \frac{\vec{r}_1 - \vec{r}_2}{2} \right) \\ + i W_{LS} \overleftarrow{\nabla}_{12} \delta(\vec{r}_1 - \vec{r}_2) \times \overrightarrow{\nabla}_{12} \cdot (\vec{\sigma}_1 + \vec{\sigma}_2)$$

### DDME Lagrangians

$$\mathcal{L}_{NN} = \overline{\Psi} \left( i\gamma^\mu \partial_\mu - M - \sum_b g_b(\rho) \phi_b \mathcal{O}_b \right) \Psi$$

$$g_i(\rho_v) = g_i(\rho_{sat}) f_i(\xi), \quad i = \sigma, \omega, \\ f_i(\xi) = a_i \frac{1 + b_i (\xi + d_i)^2}{1 + c_i (\xi + d_i)^2}, \\ g_\rho(\rho_v) = g_\rho(0) e^{-a_\rho \xi}, \\ f_\pi(\rho_v) = f_\pi(0) e^{-a_\pi \xi},$$

Non explicit  
density-dependence

### Bennaceur et al semi-regularized vertex

$$\hat{V}(x_1, x_2; x_3, x_4) = \delta(\mathbf{r}_1 - \mathbf{r}_3) \delta(\mathbf{r}_2 - \mathbf{r}_4) g_a(r_{12}) \hat{O}_j^{(n)}(\mathbf{k}_{12}, \mathbf{k}_{34}) \\ \times \left\{ W_\nu^{(n)} \hat{1}_\sigma \hat{1}_\tau + B_\nu^{(n)} \hat{P}_\sigma \hat{1}_\tau - H_\nu^{(n)} \hat{1}_\sigma \hat{P}_\tau - M_\nu^{(n)} \hat{P}_\sigma \hat{P}_\tau \right\}$$

$$\hat{V} = W_3 (\hat{V}_1 + \hat{V}_2)$$

$$\hat{V}_1 = \hat{1}_r \hat{1}_q \hat{1}_\sigma g_{a3}(\mathbf{r}_1 - \mathbf{r}_2) \delta(\mathbf{r}_2 - \mathbf{r}_3),$$

$$\hat{V}_2 = \hat{1}_r \hat{1}_q \hat{P}_{23}^\sigma g_{a3}(\mathbf{r}_1 - \mathbf{r}_2) \delta(\mathbf{r}_2 - \mathbf{r}_3).$$

### NL Lagrangians

$$\mathcal{L}_{NN} = \overline{\Psi} \left( i\gamma^\mu \partial_\mu - M - \sum_b g_b \phi_b \mathcal{O}_b \right) \Psi - U[\sigma]$$

$$U[\sigma] = \frac{1}{2} m_\sigma^2 \sigma^2 + \frac{g_2}{3} \sigma^3 + \frac{g_3}{4} \sigma^4$$

$$\mathcal{L}_{NN}^\sigma = [g_\sigma \overline{\Psi} \sigma \Psi] (x), \quad \mathcal{L}_{NN}^\pi = \left[ \frac{f_\pi(\rho_v)}{m_\pi} \overline{\Psi} \gamma^5 \gamma^\mu \partial_\mu \vec{\pi} \star \vec{\tau} \Psi \right] (x)$$

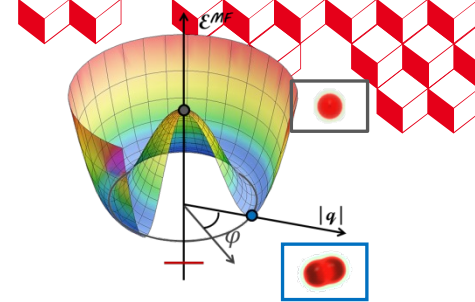
$$\mathcal{L}_{NN}^\omega = [g_\omega \overline{\Psi} \gamma^\mu \omega_\mu \Psi] (x),$$

$$\mathcal{L}_{NN}^\rho = [g_\rho \overline{\Psi} \gamma^\mu \vec{\rho}_\mu \star \vec{\tau} \Psi] (x), \quad \mathcal{L}_{NN}^{\omega+\rho;\tau} = \left[ \overline{\Psi} \sigma^{\mu\nu} \left( -\frac{g_\omega^\tau}{2M} \Omega_{\mu\nu} - \frac{g_\rho^\tau}{2M} \vec{\mathcal{R}}_{\mu\nu} \star \vec{\tau} \right) \Psi \right] (x)$$

--> Simple form  $\Leftrightarrow$  Fermi-liquid fixed point to be grasped via RG techniques ?

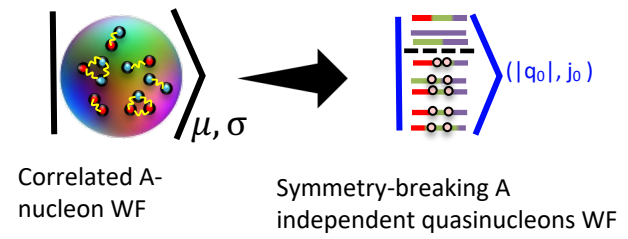


# 2 Lessons from empirical EDFs : Lesson 2



Lesson n°2 : GS + low-lying collective excited states via horizontal expansion

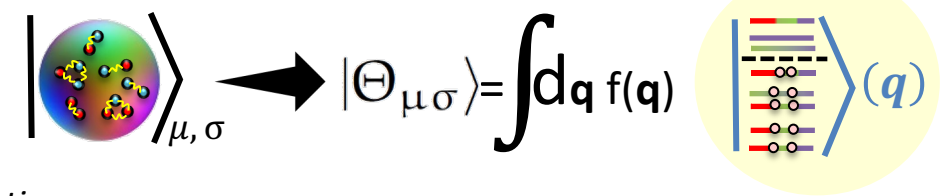
◆ dHFB treatment



*dHFB constrained calculations*

◆ Post-HFB treatment : PGCM

--> Symmetry-conserving (non orthogonal) mixture of symmetry-breaking HFB vacua

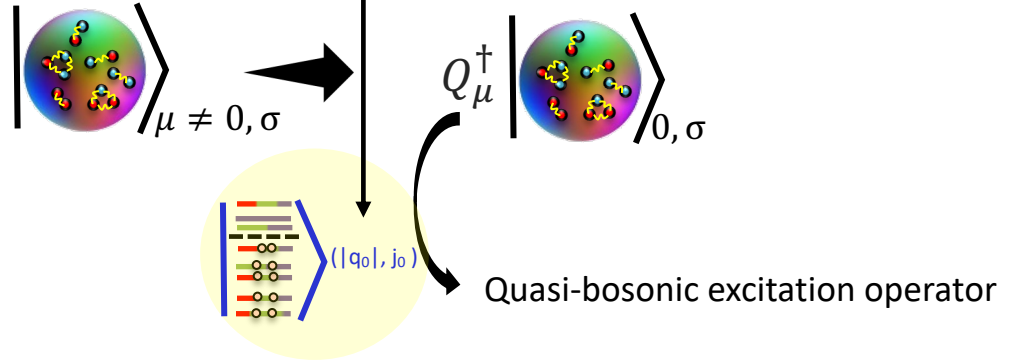


*dHFB calculation*

◆ Post-HFB : QRPA

--> Excitations = coherent mixture of 2-qp excitations

--> Harmonic limit of the GCM



--> Static correlations : fluctuations of bosonic order parameters  
 $\Rightarrow$  (Partially-)bosonizing the theory ?

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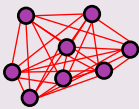

## 3 Towards a rigorous formulation of nuclear EDFs

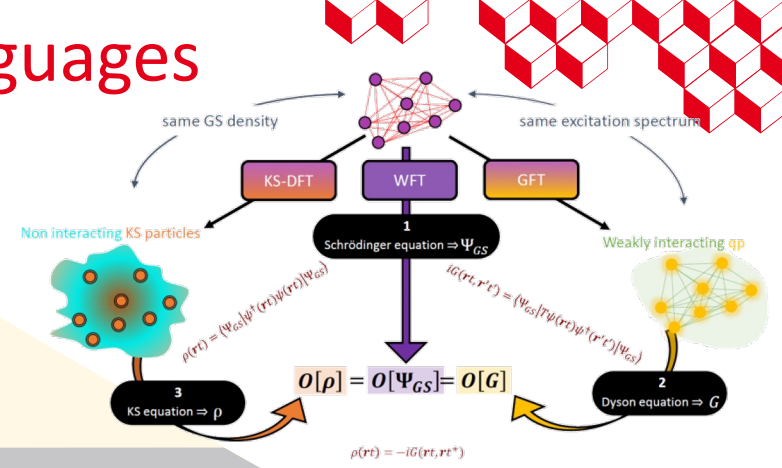
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# 3 Towards a rigorous formulation of nuclear EDFs : Languages

	Wave Function theories	Functional theories																
																		
Based on	wave function $ \Psi\rangle$	reduced quantity $\rho$																
Observables	$O[ \Psi\rangle] = \langle\Psi O \Psi\rangle$	$F[\rho]$																
		<table border="1"> <tr> <td><math>\rho</math></td> <td><math>G(\mathbf{r}, \mathbf{r}'; t - t')</math></td> <td><math>\gamma(\mathbf{r}, \mathbf{r}') = G(\mathbf{r}, \mathbf{r}'; t - t^+)</math></td> <td><math>\rho(\mathbf{r}) = \gamma(\mathbf{r}, \mathbf{r})</math></td> </tr> <tr> <td>Functional</td> <td><math>\Phi_{LW}[G]</math> or <math>\Sigma = \frac{\delta\Phi_{LW}}{\delta G}</math></td> <td><math>E_{xc}[\gamma]</math></td> <td><math>E_{xc}[\rho]</math> or <math>v_{xc} = \frac{\delta E_{xc}}{\delta\rho}</math></td> </tr> <tr> <td>Approx.</td> <td>"easy"</td> <td>difficult</td> <td>very difficult</td> </tr> <tr> <td>Computationally</td> <td>heavy</td> <td>moderate</td> <td>light</td> </tr> </table>	$\rho$	$G(\mathbf{r}, \mathbf{r}'; t - t')$	$\gamma(\mathbf{r}, \mathbf{r}') = G(\mathbf{r}, \mathbf{r}'; t - t^+)$	$\rho(\mathbf{r}) = \gamma(\mathbf{r}, \mathbf{r})$	Functional	$\Phi_{LW}[G]$ or $\Sigma = \frac{\delta\Phi_{LW}}{\delta G}$	$E_{xc}[\gamma]$	$E_{xc}[\rho]$ or $v_{xc} = \frac{\delta E_{xc}}{\delta\rho}$	Approx.	"easy"	difficult	very difficult	Computationally	heavy	moderate	light
$\rho$	$G(\mathbf{r}, \mathbf{r}'; t - t')$	$\gamma(\mathbf{r}, \mathbf{r}') = G(\mathbf{r}, \mathbf{r}'; t - t^+)$	$\rho(\mathbf{r}) = \gamma(\mathbf{r}, \mathbf{r})$															
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- 1) Nucleus: A interacting, structure-less nucleons
- 2) Structure & dynamic encoded in Hamiltonian, Functional, ...
- 3) Solve master equation to desired accuracy

$$H(\dots)|\Psi_{\mu,\sigma}\rangle = E_{\mu\tilde{\sigma}}|\Psi_{\mu,\sigma}\rangle$$

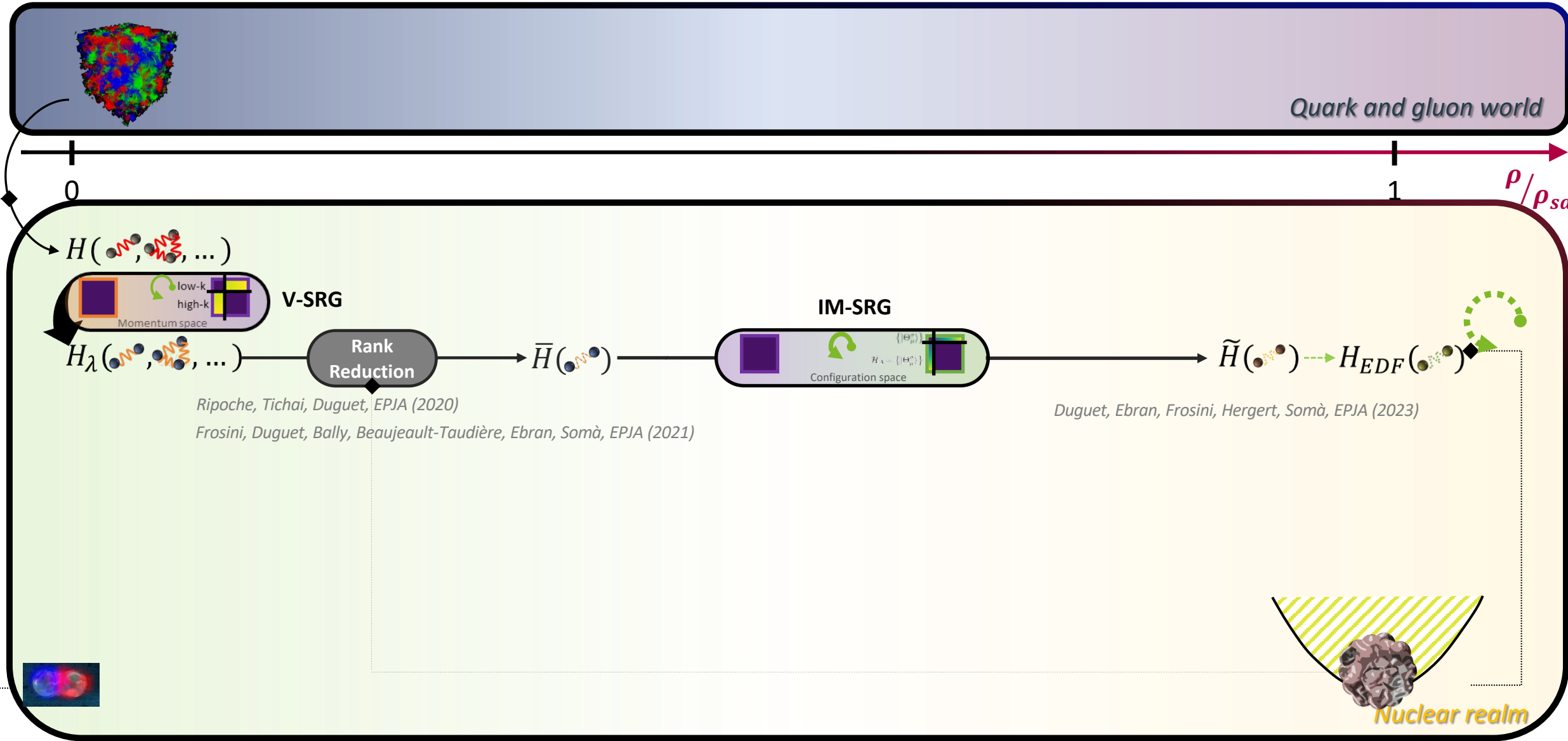
$$G^{-1}(x, x') = G_0^{-1}(x, x') - \Sigma(x, x')$$

$$h(\mathbf{r})f_\alpha(x) + \int dx' \Sigma(x, x'; \varepsilon_\alpha) f_\alpha(x') = \varepsilon_\alpha f_\alpha(x)$$

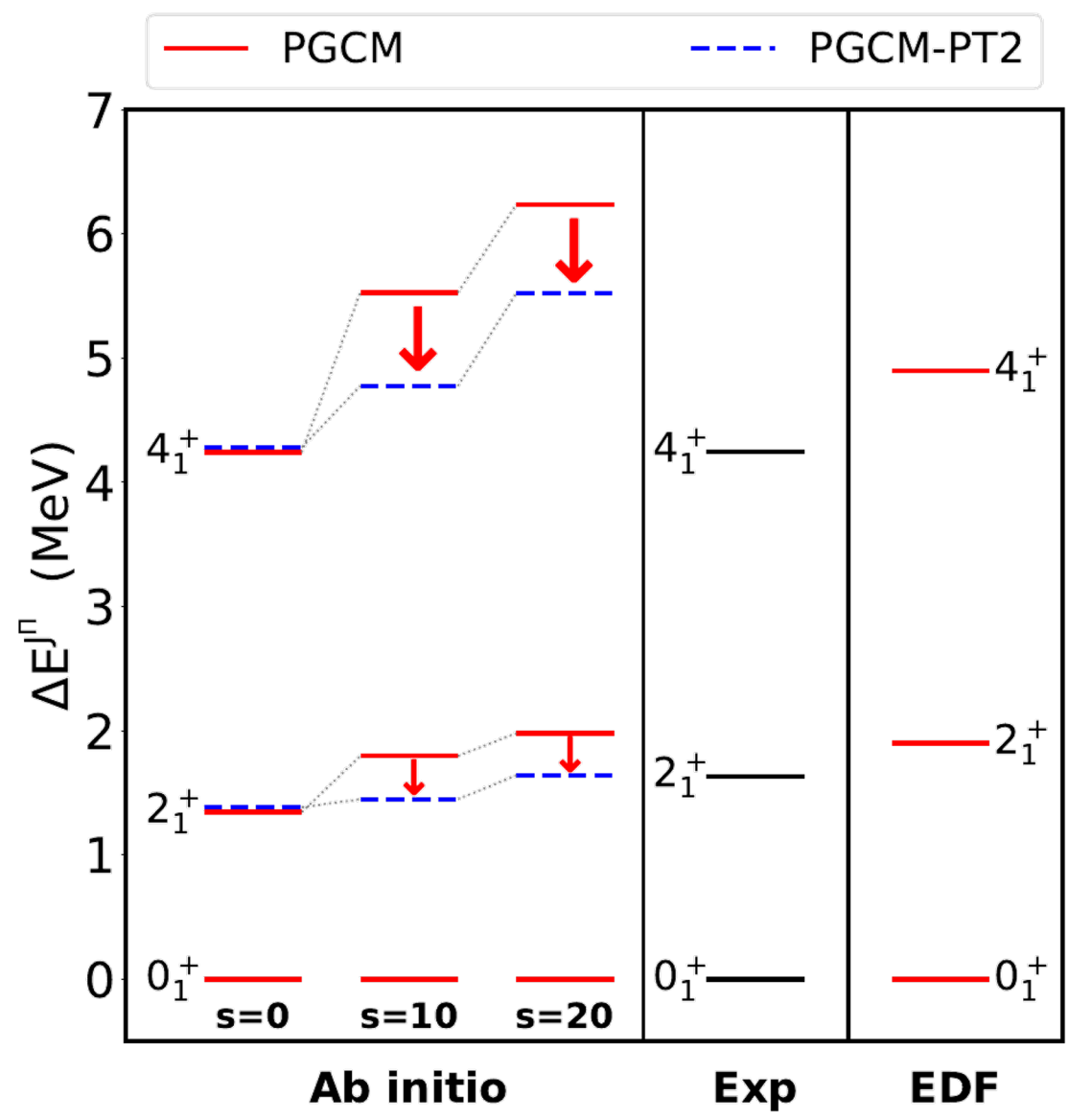
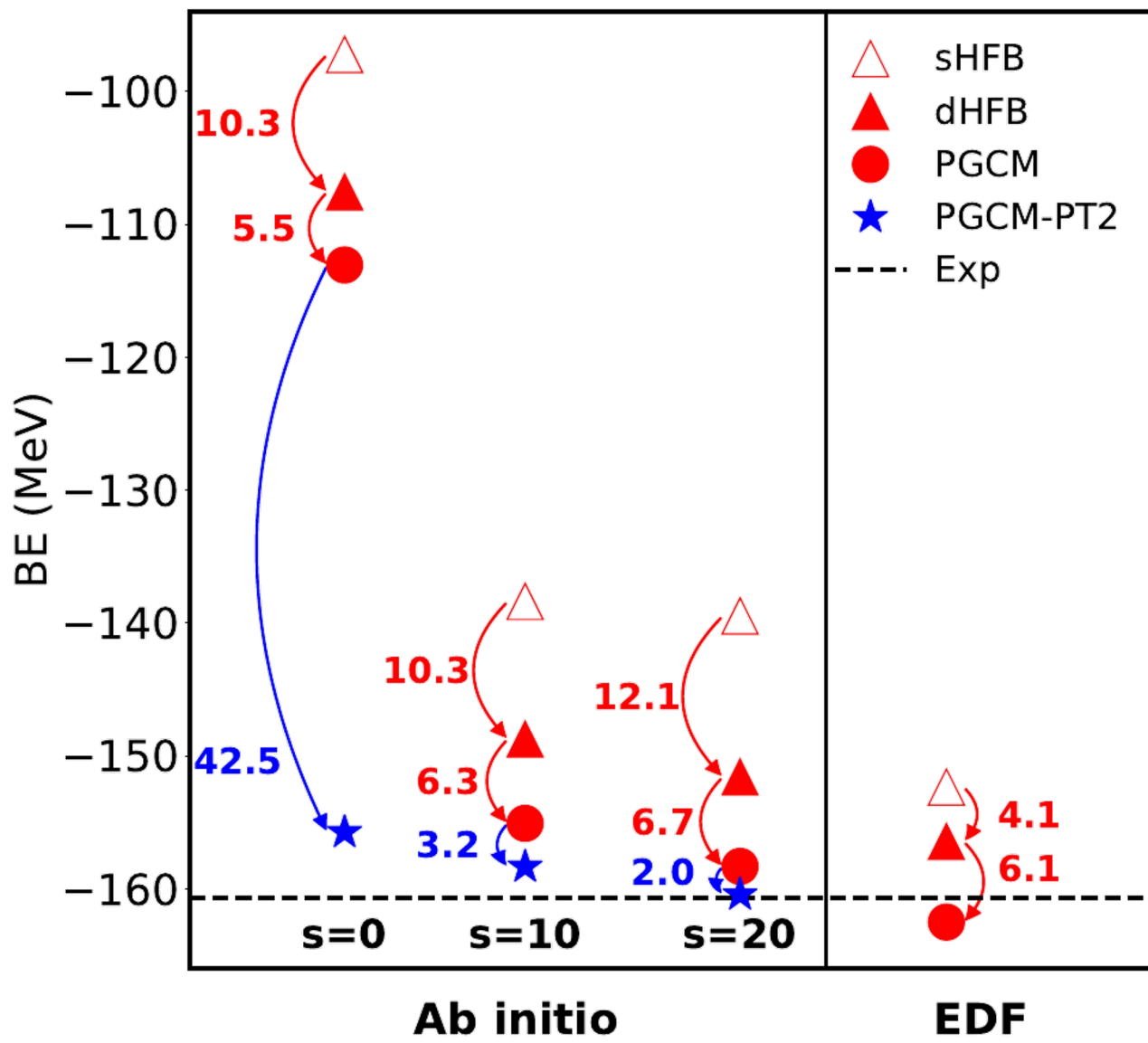
$$E_{\text{gs}} = \min_{\gamma \in \mathcal{N}\text{-rep}} E[\gamma]$$

$$\left\{ -\frac{\nabla^2}{2m} + v_{\text{KS}}(\mathbf{r}) \right\} \phi_k(\mathbf{r}) = \varepsilon_k \phi_k(\mathbf{r})$$

# 3 Towards a rigorous formulation of nuclear EDFs : WFT perspective

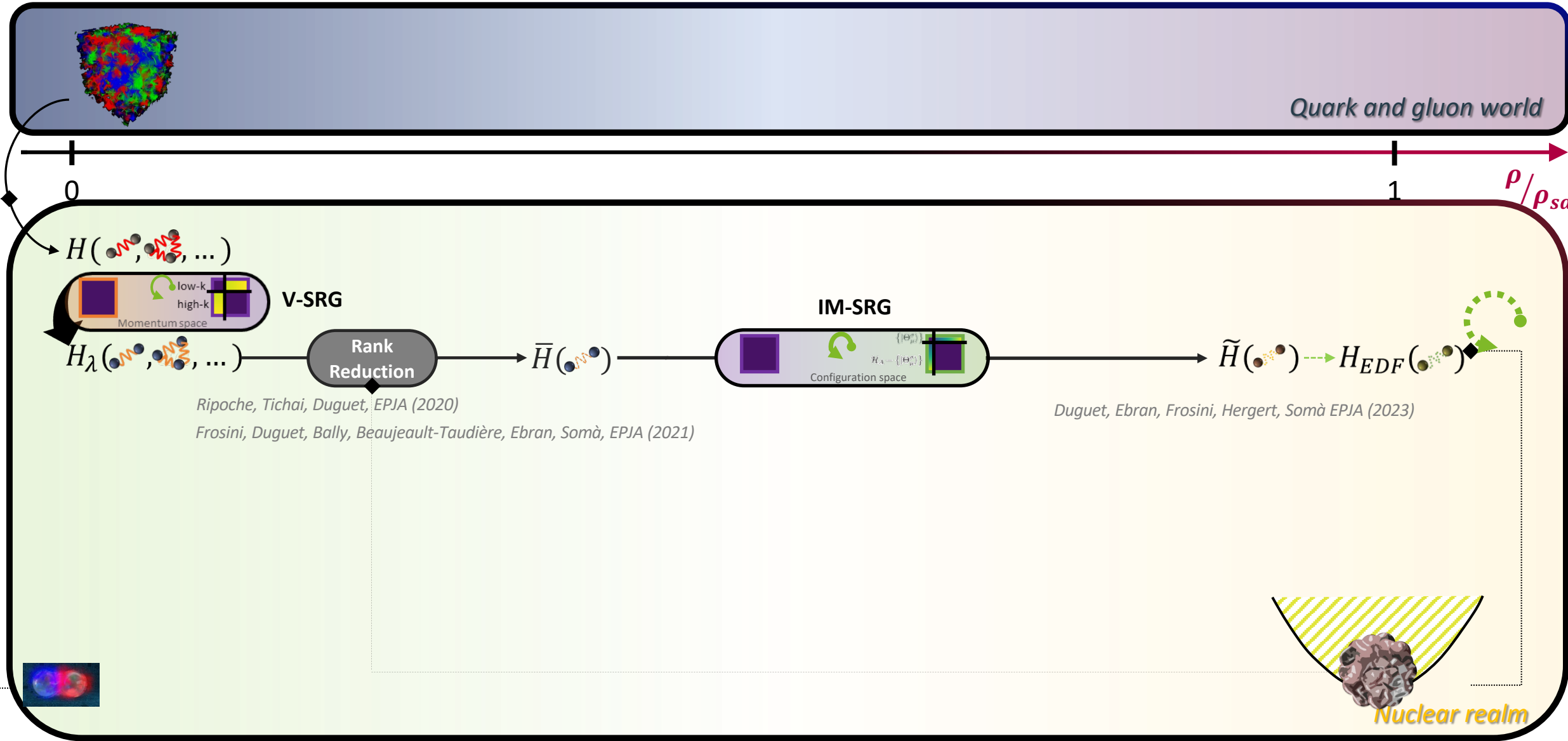


### 3 Towards a rigorous formulation of nuclear EDFs : WFT perspective





# 3 Towards a rigorous formulation of nuclear EDFs : WFT perspective



### 3 Towards a rigorous formulation of nuclear EDFs : DFT perspective

⊙ All the information needed to compute GS properties is encoded in a simple variable: the constituent density

$$H = T + v + V,$$

i) GS density uniquely defines the system.

In particular, there exists an energy (HK) functional yielding the exact GS energy when evaluated at the exact GS density :

$$\begin{aligned} E_v^{\text{HK}}[\rho(\mathbf{r})] &= \langle \Psi[\rho] | H[v[\rho], N[\rho]] | \Psi[\rho] \rangle \\ &= \langle \Psi[\rho] | T[N[\rho]] + V[N[\rho]] | \Psi[\rho] \rangle \\ &+ \int d^3r \rho(\mathbf{r}) v([\rho], \mathbf{r}) \\ &\equiv F^{\text{HK}}[\rho(\mathbf{r})] + \int d^3r \rho(\mathbf{r}) v([\rho], \mathbf{r}). \end{aligned}$$

ii) The exact GS density can be obtained via a variational principle :

$$E_{\text{gs}} = \min_{\rho \in \mathfrak{A}_N} E_v^{\text{HK}}[\rho] \quad \left. \begin{array}{l} \rho_1 \in \mathfrak{A}_N \\ \rho_2 \in \mathfrak{A}_N \end{array} \right\} \xrightarrow{?} \delta \rho_1 + (1 - \delta) \rho_2 \in \mathfrak{A}_N$$

*(Non convex) set of densities originating from a GS WF of some N-particle system subject to a given external potential*

$$E_{\text{gs}} = \min_{\rho \in \mathfrak{A}_N} \min_{\Psi \rightarrow \rho} \langle \Psi | H | \Psi \rangle \quad \mathfrak{A}_N \subset \mathfrak{A}_N$$

*(Convex) set of densities originating from arbitrary WFs with finite kinetic energy, satisfying Pauli principle and  $\int d^3r \rho(\mathbf{r}) = N$*

$$\begin{aligned} &= \min_{\rho \in \mathfrak{A}_N} \left\{ \left[ \min_{\Psi \rightarrow \rho} \langle \Psi | T + V | \Psi \rangle \right] + \int d^3r \rho(\mathbf{r}) v([\rho], \mathbf{r}) \right\} \\ &\equiv \min_{\rho \in \mathfrak{A}_N} \left\{ F^{\text{L}}[\rho] + \int d^3r \rho(\mathbf{r}) v([\rho], \mathbf{r}) \right\}. \end{aligned}$$

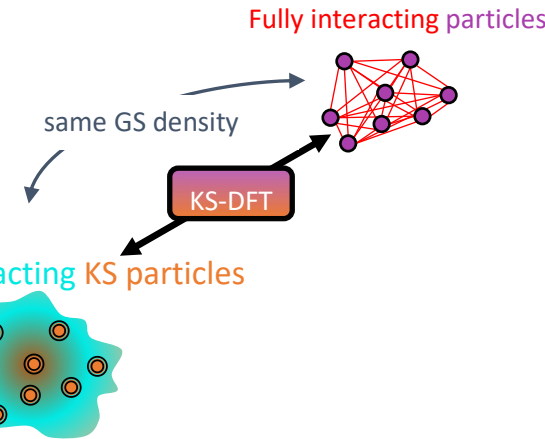
### 3 Towards a rigorous formulation of nuclear EDFs : DFT perspective

◇ Let  $S[\Theta]$  be an arbitrary functional of some N-particle WF  $|\Theta\rangle$  whose form is less complex than the exact WF  $|\Psi\rangle$ .

◇ Let  $F^S[\rho]$  be a functional of the density :  $F^S[\rho] = \min_{\Theta \rightarrow \rho} S[\Theta]$        $\rho(\mathbf{r}) = \langle \Theta | \hat{\rho}(\mathbf{r}) | \Theta \rangle$        $\hat{\rho}(\mathbf{r}) = \sum_i^N \delta(\hat{\mathbf{r}} - \mathbf{r}_i)$

◇ Let us call  $R^S[\rho] \equiv F^L[\rho] - F^S[\rho]$  the difference (remainder) between the Levy functional and the previous functional

◇ The GS energy reads:  $E_{gs} = \min_{\rho \in \mathfrak{M}_N} \left\{ F^L[\rho] + \int d^3r \rho(\mathbf{r}) v([\rho], \mathbf{r}) \right\} = \min_{\rho \in \mathfrak{M}_N} \left\{ F^S[\rho] + R^S[\rho] + \int d^3r \rho(\mathbf{r}) v(\mathbf{r}) \right\} = \min_{\rho \in \mathfrak{M}_N} \left\{ \left[ \min_{\Theta \rightarrow \rho} S[\Theta] \right] + R^S[\rho] + \int d^3r \rho(\mathbf{r}) v(\mathbf{r}) \right\}$



#### KS choice $|\Theta\rangle = |\Phi\rangle$

$$\rho \in \mathfrak{M}_N \cap \mathfrak{M}_N^0$$

$$\rho(\mathbf{r}) = \sum_i |\phi_i(\mathbf{r})|^2$$

$$E_{gs} = \min_{\rho \in \mathfrak{M}_N} \left\{ \left[ \min_{\Phi \rightarrow \rho} S[\Phi] \right] + R^S[\rho] + \int d^3r \rho(\mathbf{r}) v(\mathbf{r}) \right\}$$

$$= \min_{\{\phi_i\} \rightarrow N} \left\{ S[\{\phi_i\}] + R^S[\rho[\{\phi_i\}]] + \int d^3r \rho([\{\phi_i\}]; \mathbf{r}) v(\mathbf{r}) \right\}$$

$$\frac{\delta S[\{\phi_i\}]}{\delta \phi_k^\dagger(\mathbf{r})} + \left\{ \frac{\delta R^S[\rho]}{\delta \rho(\mathbf{r})} + v(\mathbf{r}) \right\} \phi_k(\mathbf{r}) = \varepsilon_k \phi_k(\mathbf{r})$$

#### Standard KS

$$S[\Phi] = \langle \Phi | T | \Phi \rangle = E_k[\{\phi_i\}]$$

$$R^S[\rho] = E_d[\rho] + E_x[\rho] + E_c[\rho]$$

$$E_d[\rho] \equiv \frac{1}{2} \int d^3r d^3r' V(\mathbf{r}, \mathbf{r}') \rho(\mathbf{r}) \rho(\mathbf{r}')$$

$$E_x[\rho] \equiv -\frac{1}{2} \sum_{ij} \int d^3r d^3r' V(\mathbf{r}, \mathbf{r}') \phi_i^*(\mathbf{r}) \phi_j^*(\mathbf{r}') \phi_i(\mathbf{r}') \phi_j(\mathbf{r})$$

$$E_c[\rho] \equiv F^L[\rho] - E_k[\rho] - E_d[\rho] - E_x[\rho].$$

$$\left\{ -\frac{\nabla^2}{2m} + v_{KS}(\mathbf{r}) \right\} \phi_k(\mathbf{r}) = \varepsilon_k \phi_k(\mathbf{r})$$

$$v_{KS}(\mathbf{r}) \equiv v(\mathbf{r}) + \left( \int d^3r' V(\mathbf{r}, \mathbf{r}') \rho(\mathbf{r}') \right) + \frac{\delta(E_x[\rho] + E_c[\rho])}{\delta \rho(\mathbf{r})}$$

#### Generalized KS

$$S[\Phi] = \langle \Phi | T + V | \Phi \rangle$$

$$= E_k[\{\phi_i\}] + E_d[\{\phi_i\}] + E_x[\{\phi_i\}]$$

$$R^S[\rho] = E_c[\rho]$$

$$\left\{ -\frac{\nabla^2}{2m} + v(\mathbf{r}) + \left( \int d^3r' V(\mathbf{r}, \mathbf{r}') \rho(\mathbf{r}') \right) + \frac{\delta E_c[\rho]}{\delta \rho(\mathbf{r})} \right\} \phi_k(\mathbf{r}) - \left[ \int d^3r' V(\mathbf{r}, \mathbf{r}') \left( \sum_j \phi_j^*(\mathbf{r}') \phi_j(\mathbf{r}') \right) \phi_k(\mathbf{r}') \right] = \varepsilon_k \phi_k(\mathbf{r}).$$



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**KS choice**  $|\Theta\rangle = |\Phi\rangle$

$$\rho \in \mathfrak{M}_N \cap \mathfrak{M}_N^0$$

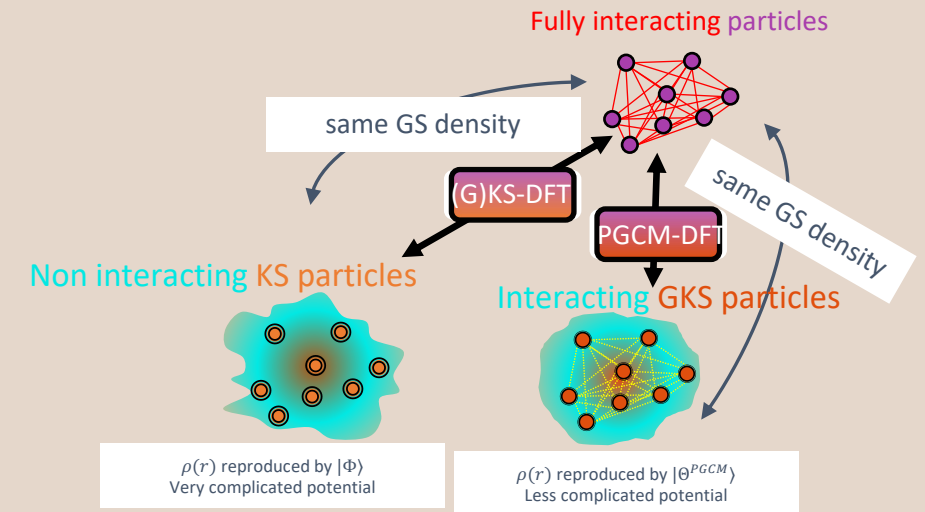
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$$= \min_{\{\phi_i\} \rightarrow N} \left\{ S[\{\phi_i\}] + R^S[\rho[\{\phi_i\}]] + \int d^3r \rho[\{\phi_i\}; \mathbf{r}] v(\mathbf{r}) \right\}$$

$$\frac{\delta S[\{\phi_i\}]}{\delta \phi_k^\dagger(\mathbf{r})} + \left\{ \frac{\delta R^S[\rho]}{\delta \rho(\mathbf{r})} + v(\mathbf{r}) \right\} \phi_k(\mathbf{r}) = \varepsilon_k \phi_k(\mathbf{r})$$

**PGCM choice**  $|\Theta\rangle = |\Theta^{PHFB/PGCM}\rangle$



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◇ Let  $F^S[\rho]$  be a functional of the density :  $F^S[\rho] = \min_{\Theta \rightarrow \rho} S[\Theta]$        $\rho(\mathbf{r}) = \langle \Theta | \hat{\rho}(\mathbf{r}) | \Theta \rangle$        $\hat{\rho}(\mathbf{r}) = \sum_i^N \delta(\hat{\mathbf{r}} - \mathbf{r}_i)$

◇ Let us call  $R^S[\rho] \equiv F^L[\rho] - F^S[\rho]$  the difference (remainder) between the Levy functional and the previous functional

◇ The GS energy reads:  $E_{gs} = \min_{\rho \in \mathfrak{M}_N} \left\{ F^L[\rho] + \int d^3r \rho(\mathbf{r}) v(\mathbf{r}) \right\} = \min_{\rho \in \mathfrak{M}_N} \left\{ F^S[\rho] + R^S[\rho] + \int d^3r \rho(\mathbf{r}) v(\mathbf{r}) \right\} = \min_{\rho \in \mathfrak{M}_N} \left\{ \left[ \min_{\Theta \rightarrow \rho} S[\Theta] \right] + R^S[\rho] + \int d^3r \rho(\mathbf{r}) v(\mathbf{r}) \right\}$

**KS choice**  $|\Theta\rangle = |\Phi\rangle$

$$\rho \in \mathfrak{M}_N \cap \mathfrak{M}_N^0$$

$$\rho(\mathbf{r}) = \sum_i |\phi_i(\mathbf{r})|^2$$

$$E_{gs} = \min_{\rho \in \mathfrak{M}_N} \left\{ \left[ \min_{\Phi \rightarrow \rho} S[\Phi] \right] + R^S[\rho] + \int d^3r \rho(\mathbf{r}) v(\mathbf{r}) \right\}$$

$$= \min_{\{\phi_i\} \rightarrow N} \left\{ S[\{\phi_i\}] + R^S[\rho[\{\phi_i\}]] + \int d^3r \rho[\{\phi_i\}; \mathbf{r}] v(\mathbf{r}) \right\}$$

$$\frac{\delta S[\{\phi_i\}]}{\delta \phi_k^\dagger(\mathbf{r})} + \left\{ \frac{\delta R^S[\rho]}{\delta \rho(\mathbf{r})} + v(\mathbf{r}) \right\} \phi_k(\mathbf{r}) = \varepsilon_k \phi_k(\mathbf{r})$$

**PGCM choice**  $|\Theta\rangle = |\Theta^{PHFB/PGCM}\rangle$

$$|\Theta_{\mu}^{JM}\rangle = \sum_q f_{\mu q}^J \frac{P_{M0N_0Z_0}^J |\Phi_q\rangle}{\sqrt{\langle \Phi_q | P_{M0N_0Z_0}^J | \Phi_q \rangle}}$$

$$\equiv \sum_q f_{\mu q}^J |JMq\rangle.$$

$$\rho^{JM\mu}(\mathbf{r}) = \langle \Theta_{\mu}^{JM} | \hat{\rho}(\mathbf{r}) | \Theta_{\mu}^{JM} \rangle$$

$$= \sum_{qq'} f_{\mu q}^{J*} \langle JMq | \hat{\rho}(\mathbf{r}) | JMq' \rangle f_{\mu q'}$$



### 3 Towards a rigorous formulation of nuclear EDFs : PI perspective

© Wightman/Schwinger reconstruction theorem : sequence of (tempered) n-point correlation functions completely determines Hilbert space and algebra of fields (up to unitary equivalence) of a given quantum system.

→ Canonical formulation :  $G_{I_1, I_2, \dots, I_n}^{(n)} \equiv \langle vac | T \hat{\varphi}_{I_1} \hat{\varphi}_{I_2} \cdots \hat{\varphi}_{I_n} | vac \rangle$

→ Path integral formulation :  $S_J[\tilde{\varphi}] = S[\tilde{\varphi}] - J_I \tilde{\varphi}_I$

$$J_I \tilde{\varphi}_I \equiv J_{x,a} \tilde{\varphi}_{x,a} \\ \equiv \sum_{m_s, c, a} \int_0^\beta d\tau \int_{\mathbb{R}^{D-1}} d^{D-1}r J_{m_s, c, a}(\tau, \mathbf{r}) \tilde{\varphi}_{m_s, -c, a}(\tau, \mathbf{r})$$

$$Z[J] = \mathcal{N} \int_{\mathcal{C}} \mathcal{D}\tilde{\varphi} e^{-\frac{1}{\hbar} S_J[\tilde{\varphi}]} \equiv e^{\frac{1}{\hbar} W[J]}$$

$$G_{I_1, I_2, \dots, I_n}^{(n)} \equiv \langle \tilde{\varphi}_{I_1} \tilde{\varphi}_{I_2} \cdots \tilde{\varphi}_{I_n} \rangle_{vac} = \frac{\int \mathcal{D}\tilde{\varphi} \tilde{\varphi}_{I_1} \tilde{\varphi}_{I_2} \cdots \tilde{\varphi}_{I_n} e^{-\frac{1}{\hbar} S[\tilde{\varphi}]}}{\int \mathcal{D}\tilde{\varphi} e^{-\frac{1}{\hbar} S[\tilde{\varphi}]}} \\ = \frac{\hbar^n}{Z[0]} \left. \frac{\delta^n Z[J]}{\delta J_{I_1} \delta J_{I_2} \cdots \delta J_{I_n}} \right|_{J=0}.$$

$$G_{I_1, I_2, \dots, I_n}^{(n), c} = \hbar^{n-1} \left. \frac{\delta^n W[J]}{\delta J_{I_1} \delta J_{I_2} \cdots \delta J_{I_n}} \right|_{J=0}$$



### 3 Towards a rigorous formulation of nuclear EDFs : PI perspective

Compact way of representing the partition function : Effective action

Classical action

$$S_{JKL^{(3)}...L^{(m)}}[\tilde{\varphi}] \equiv S[\tilde{\varphi}] - J_I \tilde{\varphi}_I - \frac{1}{2} K_{IJ} \tilde{\varphi}_I \tilde{\varphi}_J - \dots - \frac{1}{3!} L_{IJK}^{(3)} \tilde{\varphi}_I \tilde{\varphi}_J \tilde{\varphi}_K - \dots - \frac{1}{m!} L_{I_1 \dots I_m}^{(m)} \tilde{\varphi}_{I_1} \dots \tilde{\varphi}_{I_m}$$

Partition function

$$Z[J, K, L^{(3)}, \dots] \equiv e^{\frac{1}{\hbar} W[J, K, L^{(3)}, \dots]} = \mathcal{N} \int_{\mathcal{C}} \mathcal{D}\tilde{\varphi} e^{-\frac{1}{\hbar} S_{JKL^{(3)}...}[\tilde{\varphi}]}$$

Quantum action

$$\Gamma[\phi, G, V, \dots] = -W[J, K, L^{(3)}, \dots] + J_I \phi_I + \frac{1}{2} K_{IJ} (\phi_I \phi_J + \hbar G_{IJ}) + \frac{1}{6} L_{IJK}^{(3)} (\phi_I \phi_J \phi_K + \hbar G_{IJ} \phi_K + \hbar G_{IK} \phi_J + \hbar G_{JK} \phi_I + \hbar^2 V_{IJK}) + \dots$$

Gap equations

$$\left. \frac{\delta \Gamma[\phi, G, V, \dots]}{\delta \phi_I} \right|_{\phi_{gs}, G_{gs}, V_{gs}, \dots} = 0,$$

$$\left. \frac{\delta \Gamma[\phi, G, V, \dots]}{\delta G_{IJ}} \right|_{\phi_{gs}, G_{gs}, V_{gs}, \dots} = 0,$$

$$\vdots$$

Quantum effective action already contains all correlation functions at tree-level : = low-energy action with all quantum fluctuations integrated out

$$E_{gs} = \lim_{\beta \rightarrow \infty} \left( -\frac{1}{\beta} \ln(Z[J=0, \dots]) \right) = \lim_{\beta \rightarrow \infty} \left( -\frac{1}{\hbar \beta} W[J=0, \dots] \right) = \lim_{\beta \rightarrow \infty} \left( \frac{1}{\hbar \beta} \Gamma^{(nPI)}[\phi = \bar{\phi}, \dots] \right)$$

$$\frac{\delta W[J, K, L^{(3)}, \dots]}{\delta J_I} = \phi_I,$$

$$\frac{\delta W[J, K, L^{(3)}, \dots]}{\delta K_{IJ}} = \frac{1}{2} [\phi_I \phi_J + \hbar G_{IJ}],$$

$$\frac{\delta W[J, K, L^{(3)}, \dots]}{\delta L_{IJK}^{(3)}} = \frac{1}{6} [\phi_I \phi_J \phi_K + \hbar G_{IJ} \phi_K + \hbar G_{IK} \phi_J + \hbar G_{JK} \phi_I + \hbar^2 V_{IJK}],$$

$$\vdots$$

When minimizing field is homogeneous :  $\phi(x) \equiv \phi = \text{cst}$

$$\Gamma[\phi] = \beta V U(\phi)$$

$$Z(T, \mu) = e^{-\beta V U_{gc}(T, \mu)}$$

$$U_{gc}(T, \mu) = U(\phi_{gs}(T, \mu), T, \mu)$$

$$p = -U_{gc}(T, \mu), \quad n = -\frac{\partial U_{gc}(T, \mu)}{\partial \mu},$$

$$s = -\frac{\partial U_{gc}(T, \mu)}{\partial T}, \quad \epsilon = -p + \mu n + T s.$$



# 3 Towards a rigorous formulation of nuclear EDFs : Computing the effective action

## Classical action

$$S[\psi^\dagger, \psi] = \int d^4x \psi^\dagger(x) \left[ \partial_t - \frac{\nabla_x^2}{2m} \right] \psi(x) + \frac{1}{2} \int d^3x d^3y dt \psi^\dagger(x, t) \psi^\dagger(y, t) V(x, y) \psi(y, t) \psi(x, t) + \dots$$

## Generator of correlations functions

$$Z[\eta^\dagger, \eta] = e^{W[\eta^\dagger, \eta]} = \int \mathcal{D}\psi^\dagger \mathcal{D}\psi e^{-S[\psi^\dagger, \psi] + \int \eta^\dagger \psi + \psi^\dagger \eta}$$

## nP(P) Effective Action

Legendre transformation

→ Couple source(s) to local field

$$Z[\eta^\dagger, \eta] = e^{W[\eta^\dagger, \eta]} = \int \mathcal{D}\psi^\dagger \mathcal{D}\psi e^{-S[\psi^\dagger, \psi] + \int \eta^\dagger \psi + \psi^\dagger \eta} \longrightarrow \text{1PI EA } \Gamma[\phi^\dagger, \phi]$$

→ Couple source(s) to bi-local composite field

$$Z[K] = e^{W[K]} = \int \mathcal{D}\psi^\dagger \mathcal{D}\psi e^{-S[\psi^\dagger, \psi] + \frac{1}{2} \int K_{xy} \psi_x^\dagger \psi_y} \longrightarrow \text{2PI EA } \Gamma[G]$$

→ Couple source(s) to local composite field

$$Z[J] = e^{W[J]} = \int \mathcal{D}\psi^\dagger \mathcal{D}\psi e^{-S[\psi^\dagger, \psi] + \frac{1}{2} \int J_x \psi_x^\dagger \psi_x} \longrightarrow \text{2PPI EA } \Gamma[\rho] = \sup \left\{ -W[J] + \frac{1}{2} \int J_x \rho_x \right\}$$

$$\rho(x) = 2 \frac{\delta W}{\delta J(x)}$$

$$E_{\text{gs}} = \lim_{\beta \rightarrow \infty} \left( \frac{1}{\beta} \Gamma^{(n\text{PI})}[\phi = \bar{\phi}, \dots] \right)$$

## Gap equation

$$\frac{\delta \Gamma}{\delta \rho(x)} = \frac{1}{2} J(x) \quad \text{2PPI EA is extremal at the exact, physical density}$$

$$\sum_i \lambda^i \Gamma_i[\rho] = - \sum_i \lambda^i W_i \left[ \sum_i \lambda^i J_i \right] + \frac{1}{2} \int \sum_i \lambda^i J_i(x) \rho(x)$$

$$\Gamma_i[\rho] = -W_i[J_0] + \frac{1}{2} \delta_{i,0} \int J_0(x) \rho(x) + \sum_{k=1}^{i-1} \int \frac{\delta W_{i-k}[J_0]}{\delta J_0(x)} J_k(x) + \sum_{m=2}^i \frac{1}{m!} \sum_{k_1, \dots, k_m \geq 1}^{k_1 + \dots + k_m \leq i} \int \frac{\delta^m W_{i-(k_1 + \dots + k_m)}[J_0]}{\delta J_0(x_1) \dots \delta J_0(x_m)} J_{k_1}(x_1) \dots J_{k_m}(x_m)$$

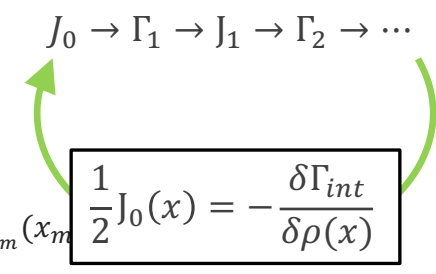
At 0<sup>th</sup> order :  $\Gamma_0[\rho] = -W_0[\rho] + \frac{1}{2} \int J_0 \rho \Rightarrow \rho(x) = 2 \frac{\delta W}{\delta J(x)} = 2 \frac{\delta W_0}{\delta J_0(x)}$

$$\frac{\delta \Gamma_0}{\delta \rho} = \cancel{\frac{1}{2} J_0} = - \int \frac{\delta W_0}{\delta J_0} \frac{\delta J_0}{\delta \rho} + \frac{1}{2} \int \frac{\delta J_0}{\delta \rho} \rho + \cancel{\frac{1}{2} J_0}$$

**$J_0(x)$  = potential reproducing the exact density  $\rho(x)$  in the non-interacting ( $\lambda = 0$ ) system !!!**

## Inversion method

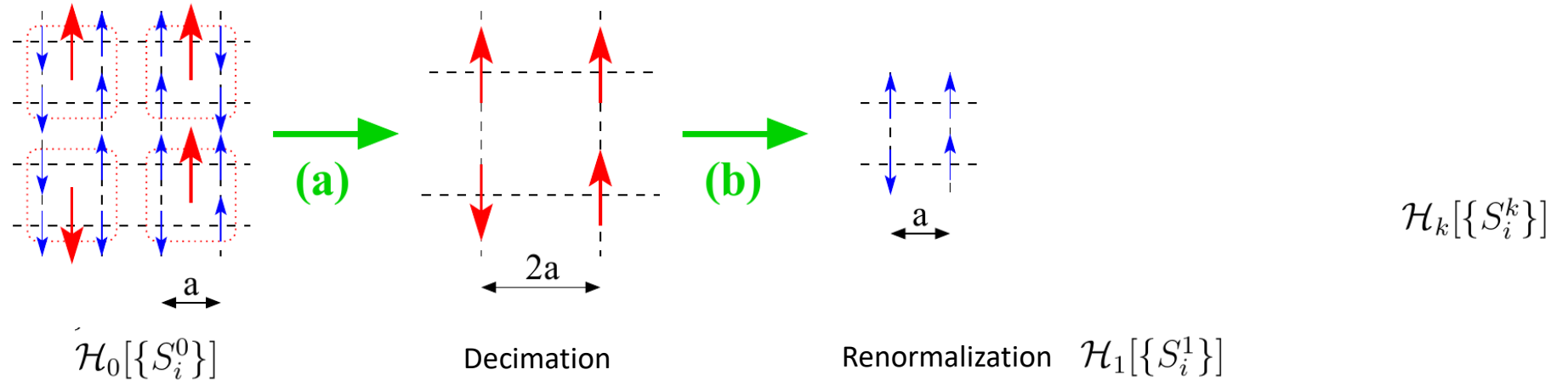
$$\left\{ \begin{aligned} \Gamma[\rho] &= \sum_i \lambda^i \Gamma_i[\rho] \\ J &= \sum_i \lambda^i J_i \\ W[J] &= \sum_i \lambda^i W_i[J] \end{aligned} \right.$$



Furnstahl, Turning the nuclear energy density functional method into a proper effective field theory: reflections. Eur. Phys. J. A 56, 85 (2020)  
 Fraboulet, Ebran, Addressing energy density functionals in the language of path-integrals I: comparative study of diagrammatic techniques applied to the (0+0)-D O(N)-symmetric  $\phi^4$ -theory. Eur. Phys. J. A 59, 91 (2023)

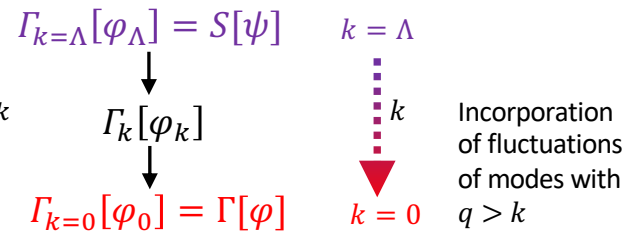
# 3 Towards a rigorous formulation of nuclear EDFs : Computing the effective action

## Renormalization group transformation : Wilson-Kadanoff procedure



## Renormalization group transformation : FRG

→ Central object of FRG : scale-dependent (or average) effective action  $\Gamma_k$  interpolating between the S and  $\Gamma$



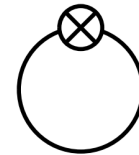
→ Mass term  $S + \Delta S_k$

$$\Delta S_k = \frac{1}{2} \int \psi^\dagger(q) R_k(q) \psi(-q)$$

→ Exact RG (or Wetterich) equation

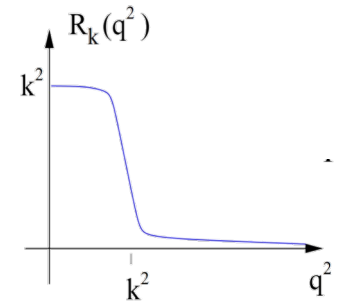
$$\partial_k \Gamma_k[\varphi] = \frac{1}{2} \text{tr} \left\{ \partial_k R_k \left( \Gamma_k^{(2)}[\varphi] + R_k \right)^{-1} \right\}$$

$$\partial_k \Gamma_k[\bar{\psi}, \psi] = - \text{tr} \left\{ \partial_k R_k \left( \Gamma_k^{(1,1)}[\bar{\psi}, \psi] + R_k \right)^{-1} \right\}$$

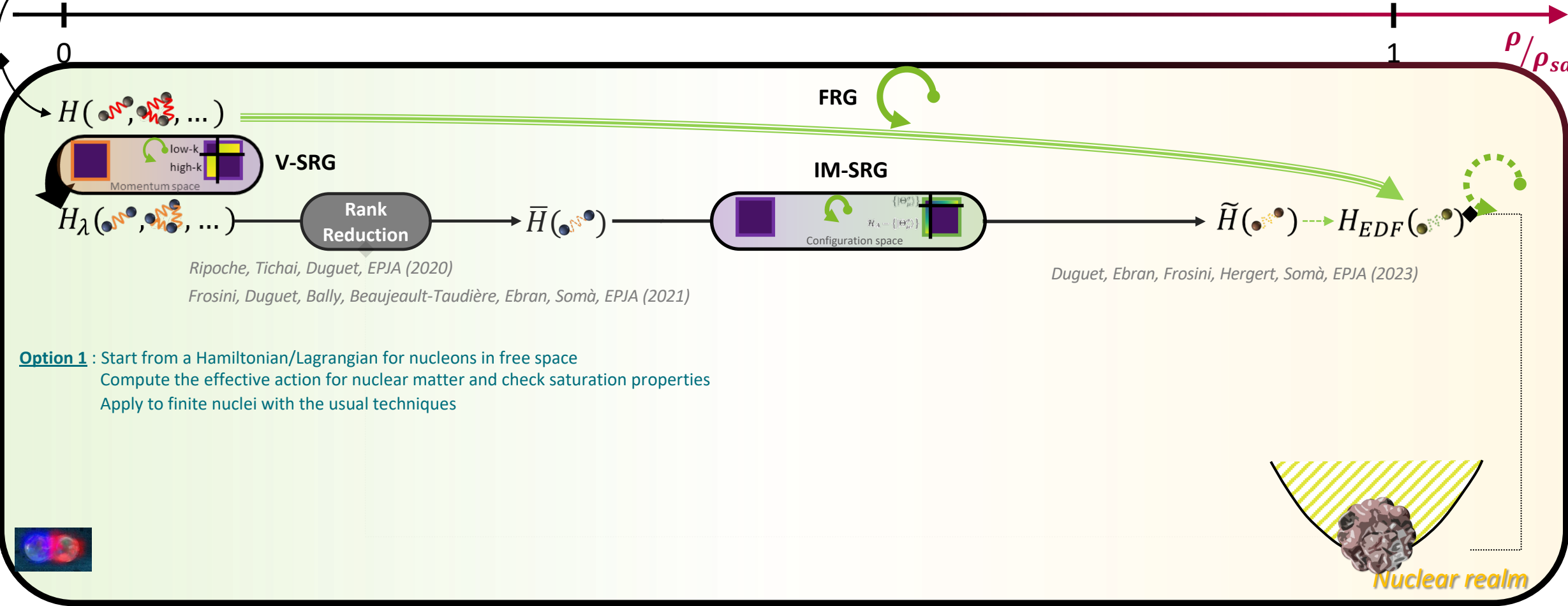


$$\Gamma_k^{(a)}[\varphi] = \frac{\delta^a}{\delta \varphi^a} \Gamma_k[\varphi]$$

$$\Gamma_k^{(a,b)}[\psi, \bar{\psi}] = \frac{\overleftarrow{\delta^a}}{\delta \psi^a} \Gamma_k[\psi, \bar{\psi}] \frac{\overleftarrow{\delta^b}}{\delta \psi^b}$$

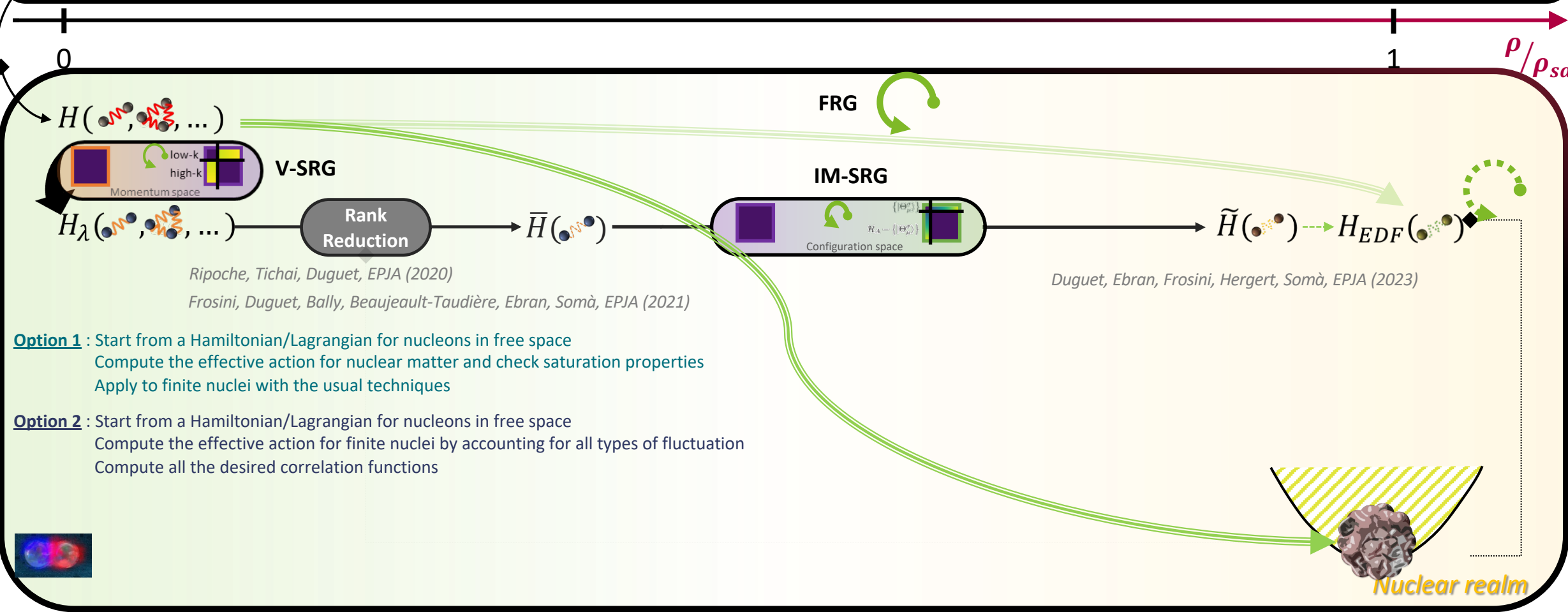


# 3 Towards a rigorous formulation of nuclear EDFs : FRG perspective





# 3 Towards a rigorous formulation of nuclear EDFs : FRG perspective

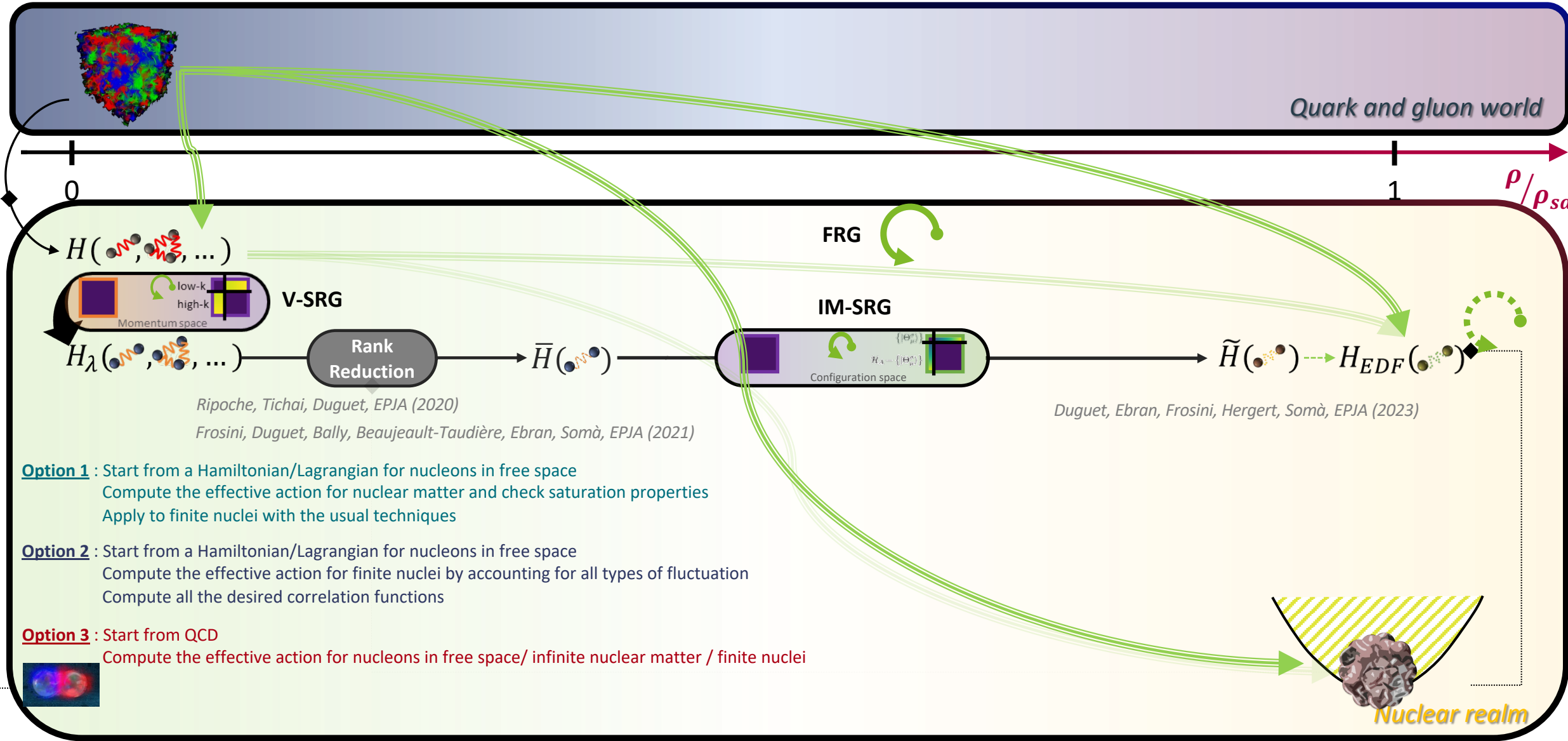


- Option 1** : Start from a Hamiltonian/Lagrangian for nucleons in free space  
 Compute the effective action for nuclear matter and check saturation properties  
 Apply to finite nuclei with the usual techniques
- Option 2** : Start from a Hamiltonian/Lagrangian for nucleons in free space  
 Compute the effective action for finite nuclei by accounting for all types of fluctuation  
 Compute all the desired correlation functions





# 3 Towards a rigorous formulation of nuclear EDFs : FRG perspective

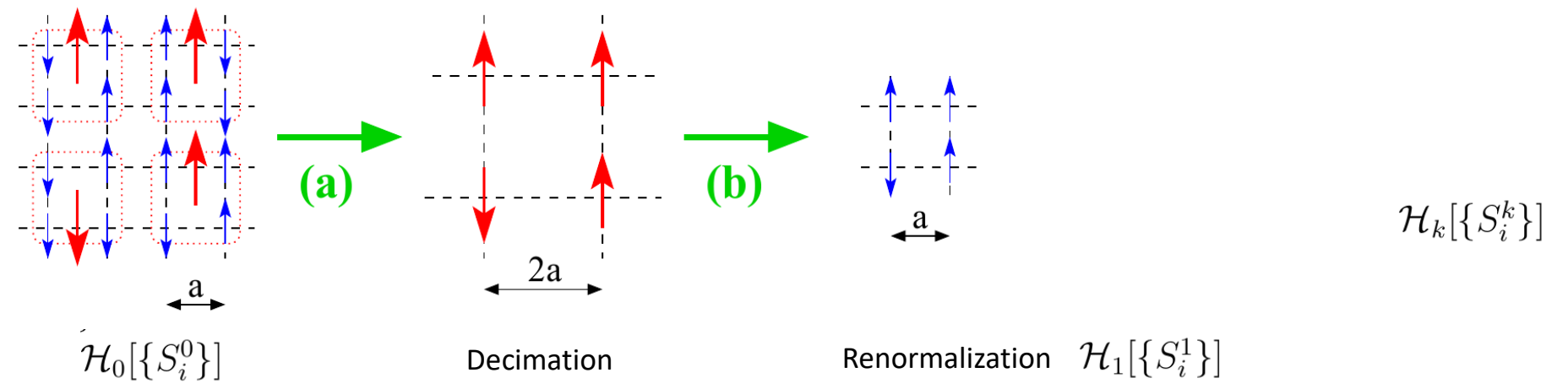


- Option 1 :** Start from a Hamiltonian/Lagrangian for nucleons in free space  
 Compute the effective action for nuclear matter and check saturation properties  
 Apply to finite nuclei with the usual techniques
- Option 2 :** Start from a Hamiltonian/Lagrangian for nucleons in free space  
 Compute the effective action for finite nuclei by accounting for all types of fluctuation  
 Compute all the desired correlation functions
- Option 3 :** Start from QCD  
 Compute the effective action for nucleons in free space/ infinite nuclear matter / finite nuclei

# 3 Towards a rigorous formulation of nuclear EDFs : FRG perspective

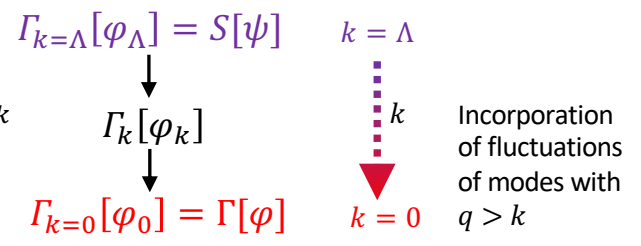


Renormalization group transformation : Wilson-Kadanoff procedure



Renormalization group transformation : FRG

Central object of FRG : scale-dependent (or average) effective action  $\Gamma_k$  interpolating between the S and  $\Gamma$



Mass term  $S + \Delta S_k$

$$\Delta S_k = \frac{1}{2} \int \psi^\dagger(q) R_k(q) \psi(-q)$$

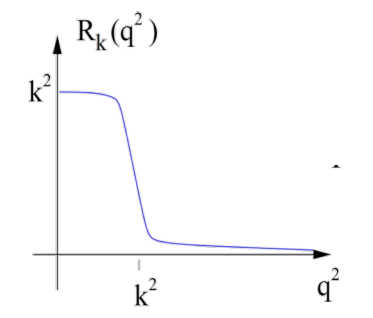
Exact RG (or Wetterich) equation

$$\partial_k \Gamma_k[\varphi] = \frac{1}{2} \text{tr} \left\{ \partial_k R_k \left( \Gamma_k^{(2)}[\varphi] + R_k \right)^{-1} \right\}$$

$$\partial_k \Gamma_k[\bar{\psi}, \psi] = - \text{tr} \left\{ \partial_k R_k \left( \Gamma_k^{(1,1)}[\bar{\psi}, \psi] + R_k \right)^{-1} \right\} = \text{ring diagram}$$

$$\Gamma_k^{(a)}[\varphi] = \frac{\delta^a}{\delta \varphi^a} \Gamma_k[\varphi]$$

$$\Gamma_k^{(a,b)}[\psi, \bar{\psi}] = \frac{\overleftarrow{\delta^a}}{\delta \psi^a} \Gamma_k[\psi, \bar{\psi}] \frac{\overleftarrow{\delta^b}}{\delta \psi^b}$$



### 3 Towards a rigorous formulation of nuclear EDFs : FRG perspective



● Truncation of the effective action

$$\Gamma_k[\Phi] = \int_x \sum_i g_{i,k} \mathcal{O}_i[\Phi]$$

$$\partial_k \Gamma_k[\bar{\psi}, \psi] = -\text{tr} \left\{ \partial_k R_k \left( \Gamma_k^{(1,1)}[\bar{\psi}, \psi] + R_k \right)^{-1} \right\} = \text{Diagram}$$

--> Derivative expansion :

- ◆ Expand in spatial derivative
- ◆ Keep all  $\Gamma_k^{(n)}$  vertex functions
- ◆ Keep the full field dependence

LPA:  $\Gamma_k = \int_x \{ U_k[\varphi] + \frac{1}{2} (\partial_\mu \varphi)^2 \}$

DE2:  $\Gamma_k = \int_x \{ U_k[\varphi] + \frac{1}{2} Z_k[\varphi] (\partial_\mu \varphi)^2 \}$

DE4 (Canet et al. '03):  $\Gamma_k = \int_x \{ U_k[\varphi] + \frac{1}{2} Z_k[\varphi] (\partial_\mu \varphi)^2 + \frac{1}{2} W_{a;k}[\varphi] (\partial_\mu \partial_\nu \varphi)^2 + \frac{1}{2} W_{b;k}[\varphi] \phi \partial^2 \phi (\partial_\mu \varphi)^2 + \frac{1}{2} W_{c;k}[\varphi] (\partial_\mu \varphi)^4 \}$

◆ Further expansion in fields  $U_k[\varphi] = \sum_i^n U_{i,k} (\varphi - \varphi_0)^i$



### 3 Towards a rigorous formulation of nuclear EDFs : FRG perspective

--> Start with a phenomenological ab initio Lagrangian

$$\begin{aligned}
 \mathcal{L}_{\text{Bonn}} = & \bar{\psi} \left[ i \not{\partial} - M - g_{\sigma} \sigma - g_{\delta} \vec{\delta} \cdot \vec{\tau} \right. \\
 & - \frac{f_{\eta}}{m_{\eta}} \gamma^5 \not{\partial} \eta - \frac{f_{\pi}}{m_{\pi}} \gamma^5 \not{\partial} \vec{\pi} \cdot \vec{\tau} \\
 & \left. - g_{\omega} \psi - \frac{f_{\omega}}{4M} \sigma^{\mu\nu} \Omega_{\mu\nu} - g_{\rho} \vec{\rho} \cdot \vec{\tau} - \frac{f_{\rho}}{4M} \sigma^{\mu\nu} \vec{R}_{\mu\nu} \cdot \vec{\tau} \right] \psi \\
 & + \frac{1}{2} (\partial_{\mu} \sigma \partial^{\mu} \sigma - m_{\sigma}^2 \sigma^2) + \frac{1}{2} (\partial_{\mu} \vec{\delta} \cdot \partial^{\mu} \vec{\delta} - m_{\delta}^2 \vec{\delta}^2) \\
 & + \frac{1}{2} (\partial_{\mu} \eta \partial^{\mu} \eta - m_{\eta}^2 \eta^2) + \frac{1}{2} (\partial_{\mu} \vec{\pi} \cdot \partial^{\mu} \vec{\pi} - m_{\pi}^2 \vec{\pi}^2) \\
 & + \frac{1}{2} \left( \frac{1}{2} \Omega^{\mu\nu} \Omega_{\mu\nu} + m_{\omega}^2 \omega^{\mu} \omega_{\mu} \right) + \frac{1}{2} \left( \frac{1}{2} \vec{R}^{\mu\nu} \cdot \vec{R}_{\mu\nu} + m_{\rho}^2 \vec{\rho}^{\mu} \cdot \vec{\rho}_{\mu} \right)
 \end{aligned}$$

--> Put it in medium : extra  $\mu \psi^{\dagger} \psi$  factor in the Lagrangian

--> Ansatz for the average effective action

$$\Gamma_k = \int d^4x \left\{ \bar{\psi} \left[ \gamma_{E}^{\mu} \partial_{\mu}^E + M + g_{\sigma;k} \sigma - \gamma_E^0 (i g_{\omega;k} \omega_0^E + \mu) \right] \psi + \frac{1}{2} \partial_{\mu}^E \sigma \partial_E^{\mu} \sigma + \mathcal{U}_k(\mu, \sigma, \omega_0^E) \right\}$$

--> Plug in Wetterich equation  $\Rightarrow$  Flow equation for effective potential + beta functions for Yukawa couplings

--> Obtain a NL-like Lagrangian

$$\begin{aligned}
 \mathcal{L}_{\text{NL}} = & \bar{\psi} \left[ i \not{\partial} - M - g_{\sigma} \sigma - \frac{f_{\pi}}{m_{\pi}} \gamma^5 \not{\partial} \vec{\pi} \cdot \vec{\tau} - g_{\omega} \psi - g_{\rho} \vec{\rho} \cdot \vec{\tau} \right] \psi \\
 & + \frac{1}{2} \partial_{\mu} \sigma \partial^{\mu} \sigma - U[\sigma] \\
 & + \frac{1}{2} \left( \frac{1}{2} \Omega^{\mu\nu} \Omega_{\mu\nu} + m_{\omega}^2 \omega^{\mu} \omega_{\mu} \right) + \frac{1}{2} \left( \frac{1}{2} \vec{R}^{\mu\nu} \cdot \vec{R}_{\mu\nu} + m_{\rho}^2 \vec{\rho}^{\mu} \cdot \vec{\rho}_{\mu} \right)
 \end{aligned}$$

$$U[\sigma] = \frac{1}{2} m_{\sigma}^2 \sigma^2 + \frac{g_2}{3} \sigma^3 + \frac{g_3}{4} \sigma^4$$

--> Check properties of nuclear matter