# Non-empirical energy functionals from low-momentum interactions

## I. Introduction to Energy Density Functional methods

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# Lecture series

## Outline

1. Introduction to energy density functional methods
   - Basics of formalism
   - Empirical energy functionals: form, performances and limitations
   - Towards non-empirical energy functionals
2. Low-momentum interactions from renormalization group methods
3. The building of non-empirical energy functionals

## Take-away message

### Theoretical methods

1. Ab-initio methods = $A$-body problem solved in terms of vacuum $H(\Lambda)$
2. Ab-initio methods limited to $A \leq 16$ plus a few doubly-magic nuclei
3. Approaches to heavier nuclei need to be benchmarked by ab-initio methods

### Energy density functional method

1. Two successive levels of implementation: single reference and multi reference
2. Empirical energy functionals successful but lack predictive power
3. Need to connect the energy functional to vacuum $H(\Lambda)$ = non-empirical EDF

# Outline

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1. Introduction
   - Basic facts about low-energy nuclear physics
   - Theoretical methods
2. Energy density functional methods
   - Sketch of the overall EDF formalism
   - Single-reference implementation: elements of formalism
   - Empirical energy functionals
   - Performances and limitations
   - Towards non-empirical energy functionals
3. Bibliography

# Outline

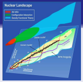
# What is low-energy nuclear physics interested in?

## In generic terms

- Spectrum of $H\,|\Psi_i^A\rangle = E_i^A\,|\Psi_i^A\rangle$ for all $A = N + Z$
- Observables for each state, e.g. $r^2 \equiv \langle\Psi_i^A|\sum_k^A \hat{r}_k^2|\Psi_i^A\rangle/A$
- Decays between $|\Psi_i\rangle$, i.e. nuclear, electromagnetic, electro-weak

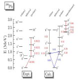
### Ground state

Mass, deformation



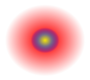

### Spectroscopy

Excitations modes



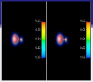
### Limits

Drip-lines, halos



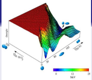
### Reaction properties

Fusion, transfer...



### Heavy elements

Fission, fusion, SHE



### Astrophysics

NS, SN, r-process

# How does that translate to low-energy nuclear theory?

## Goals for low-energy nuclear theory

1. Model the unknown nuclear Hamiltonian $H$
2. Solve $A$-body problem and describe properties of nuclei
3. Understand states of nuclear matter in astrophysical environments

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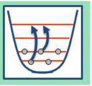
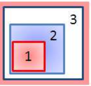
# Outline

# Which theoretical method(s)?

## Ab-initio methods

- Solve the N-body problem in terms of point-like nucleons+$H(\Lambda)$

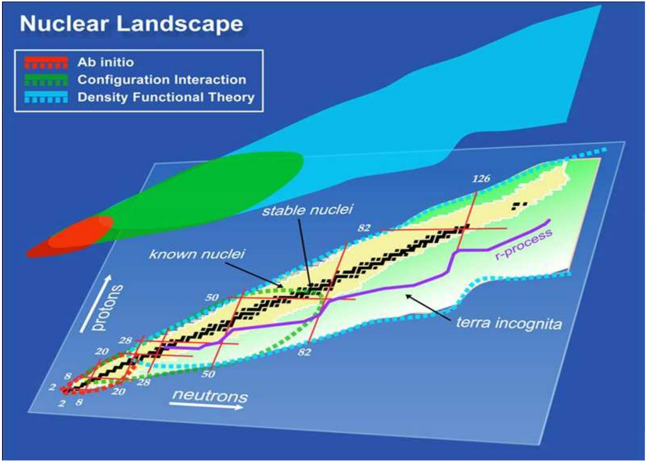
| Name | Short description | Variational | Scale as | Up to |
|---|---|---|---|---|
| Few-body (Faddeev...) | $H\Psi = E\Psi$  | Yes | $M^A$ | A = 2-4 |
| Green-Function Monte-Carlo (GFMC) | $\Psi(\tau)=e^{-(H-E_0)\tau}\Psi_T$ $=[e^{-(H-E_0)\Delta\tau}]^n\Psi_T$ + auxiliary field  | Yes | $\frac{M!}{(M-A)!A!}$ | A <12 |
| No-core Shell Model | $H\Psi = E\Psi$  | Yes | $4^A$ | A <16 |
| Coupled-Cluster (CC) | $\vert\Psi\rangle = e^S\vert\Psi_0\rangle$ $S = S_1 + S_2 + \cdots$   | No | $(M-A)^4 A^2$ | A <100 Only doubly-magic for now |

M : configuration space size

From D. Lacroix

- Limited reach over the mass table

# Which theoretical method(s)?




- No “one size fits all” theory for nuclei
- All theoretical approaches need to be linked

# Outline

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# Energy Density Functional method

## Basic elements

- Approaches not based on a correlated wave-function
- Energy is postulated to be a functional of one-body density (matrices)
- Symmetry breaking is at the heart of the method
- Two formulations (i) Single-Reference (ii) Multi-Reference

## Pros

- Use of full single-particle space
- Collective picture but fully quantal
- Universality of the EDF ($A \gtrsim 16$)
- Ground-state description
- Smoothly varying correlations

## Difficulties

- No universal parametrization
- Empirical $\neq$ predictive power
- Spectroscopy
- Fluctuating correlations with $A$
- Limited accuracy ($\sigma_{2135}^{mass} \approx 700$ keV)

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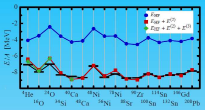
# Energy Density Functional method: single-reference implementation

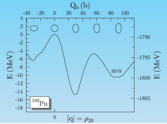
MR

## Correlations

- "Bulk" $\sim$ 800 MeV




- "Static deformation" $\sim$ 20 MeV




One auxiliary vacuum $|\Phi\rangle$

$$E = \mathcal{E}[\rho, \kappa, \kappa^*]$$

$$\rho_{ij} = \frac{\langle\Phi|a_j^\dagger a_i|\Phi\rangle}{\langle\Phi|\Phi\rangle}$$

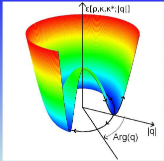
$$\kappa_{ij} = \frac{\langle\Phi|a_j a_i|\Phi\rangle}{\langle\Phi|\Phi\rangle}$$

$$\kappa_{ij}^* = \frac{\langle\Phi|a_i^\dagger a_j^\dagger|\Phi\rangle}{\langle\Phi|\Phi\rangle}$$

## Single Reference (SR)

## Broken symmetries

$N, Z, \vec{P}, J^2, J_Z, \Pi, \mathcal{T}^2$




## Hartree-Fock-Bogoliubov

## Transition probabilities

- Selection rules lost

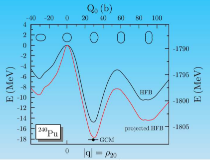
## Observables

- Binding energies
- Shell structure
- Pairing gap
- Fission barriers
- Individual excitation
- Rotational excitation

# Energy Density Functional method: multi-reference implementation

## Correlations

- "Collective fluctuations" $\sim$ 4 MeV




$$E = \sum_{AB} f_{AB}\, \mathcal{E}[\rho^{AB}, \kappa^{AB}, \kappa^{BA*}]$$

Set of auxiliary vacua $\{|\Phi_A\rangle\}$

$$\rho^{AB}_{ij} = \frac{\langle \Phi^A | a^\dagger_j a_i | \Phi^B \rangle}{\langle \Phi^A | \Phi^B \rangle}$$

$$\kappa^{AB}_{ij} = \frac{\langle \Phi^A | a_j a_i | \Phi^B \rangle}{\langle \Phi^A | \Phi^B \rangle}$$

$$\kappa^{BA*}_{ij} = \frac{\langle \Phi^A | a^\dagger_i a^\dagger_j | \Phi^B \rangle}{\langle \Phi^A | \Phi^B \rangle}$$

**Multi Reference (MR)**

SR

## Symmetry restorations

$N, Z, \vec{P}, J^2, J_Z, \Pi, \mathcal{T}^2$

## Generator Coordinate Method

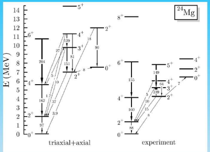
$\Delta_N, \Delta_Z, Q_{20}, Q_{30}, \cdots$

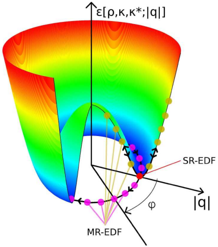
Harmonic limit → QRPA

Gaussian overlap approx. → Bohr hamiltonian

## Transition probabilities

- Selection rules restored



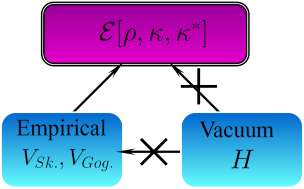

## Observables

- Same as SR
- Vibration excitations
- Rotational bands of transitional nuclei
- LACM and shape coexistence

# Energy Density Functional method: some relevant questions

**Single Reference**

Multi Reference

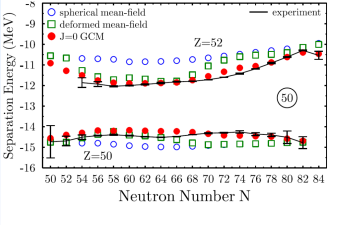



## Non empirical ?

- What form of vacuum $H$ ?
- Can we relate $\mathcal{E}[\rho, \kappa, \kappa^*]$ to $H$ ?
- Needed to go through $V_{eff.}$ ?

## Empirical knowledge

- $\mathcal{E}[\rho, \kappa, \kappa^*]$ built empirically so far
- Effective separation of scales for correlations
  - Bulk $\sim$ 800 Mev $\propto$ A
  - Collective def. $\leq$ 20 Mev $= F(N_{val}, G_{deg})$
  - Collective fluct. $\leq$ 4 MeV $= G(N_{val}, G_{deg})$
- Observables impacted by correlation
  - Symmetry breaking
  - Collective fluctuation



# Outline

# Single-reference EDF method

## Elements of formalism

- $\mathcal{E}[\rho, \kappa^*, \kappa]$ = functional of one-body density matrices

$$\rho_{ji} \equiv \langle \Phi | b_i^\dagger \, b_j | \Phi \rangle \quad ; \quad \kappa_{ji} \equiv \langle \Phi | b_i \, b_j | \Phi \rangle$$

defined in an arbitrary single-particle basis $\{b_i^\dagger ; b_i\}$

# Single-reference EDF method

## Elements of formalism

- $\mathcal{E}[\rho, \kappa^*, \kappa]$ = functional of one-body density matrices
- $|\Phi\rangle$ = auxiliary symmetry-breaking product state of reference

$$
\begin{aligned}
|\Phi\rangle &\equiv \prod_i \beta_i \, |0\rangle \\
\beta_i &\equiv \sum_i U^*_{ji} \, b_j + V^*_{ji} \, b^+_j
\end{aligned}
$$

and is a vacuum, i.e. $\beta_i \, |\Phi\rangle = 0 \;\; \forall \, i$

# Single-reference EDF method

## Elements of formalism

- $\mathcal{E}[\rho, \kappa^*, \kappa]$ = functional of one-body density matrices
- $|\Phi\rangle$ = auxiliary symmetry-breaking product state of reference
- Minimizing $\mathcal{E}[\rho, \kappa^*, \kappa]$ leads to Hartree-Fock-Bogoliubov-like equations

$$\begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^*+\lambda \end{pmatrix} \begin{pmatrix} U_i \\ V_i \end{pmatrix} = E_i \begin{pmatrix} U_i \\ V_i \end{pmatrix}$$

  - Effective potentials and vertices are defined through

$$h_{ij} \equiv \frac{\delta \mathcal{E}}{\delta \rho_{ji}} \equiv t_{ij} + \sum_{kl} \overline{v}^{ph}_{ikjl}\, \rho_{lk} \quad ; \quad \Delta_{ij} \equiv \frac{\delta \mathcal{E}}{\delta \kappa^*_{ij}} \equiv \frac{1}{2} \sum_{kl} \overline{v}^{pp}_{ijkl}\, \kappa_{kl}$$

  - $\overline{v}^{ph}/\overline{v}^{pp}$ = Consistent many-body expansion in terms of NN/NNN
  - Quasiparticle w.f. $(U_i, V_i)$, energy $E_i$, densities...

# Outline

# Empirical parameterizations of $\mathcal{E}[\rho, \kappa, \kappa^*]$ ; e.g. Skyrme or Gogny

## Local Skyrme EDF for even-even nuclei ground-state

- Density matrices expressed in position $\otimes$ spin $\otimes$ isospin s.p. basis

$$\rho_{\vec{r}\sigma q \vec{r}'\sigma' q} \equiv \langle\Phi| \, c^\dagger(\vec{r}'\sigma' q) \, c(\vec{r}\sigma q) \, |\Phi\rangle$$

$$\kappa_{\vec{r}\sigma q \vec{r}'\sigma' q} \equiv \langle\Phi| \, c(\vec{r}'\sigma' q) \, c(\vec{r}\sigma q) \, |\Phi\rangle$$

- Local densities

$$\rho_q(\vec{r}) \equiv \textstyle\sum_\sigma \rho_{\vec{r}\sigma q \vec{r}\sigma q}$$ Matter

$$\tau_q(\vec{r}) \equiv \textstyle\sum_\sigma \nabla \cdot \nabla' \rho_{\vec{r}\sigma q \vec{r}'\sigma q}\Big|_{\vec{r}=\vec{r}'}$$ Kinetic

$$J_{q,\mu\nu}(\vec{r}) \equiv \tfrac{i}{2} \textstyle\sum_{\sigma\sigma'} \left(\nabla' - \nabla\right)_\mu \rho_{\vec{r}\sigma q \vec{r}'\sigma' q} \, \sigma_\nu^{\sigma'\sigma}\Big|_{\vec{r}=\vec{r}'}$$ Spin-current tensor

$$J_{q,\kappa}(\vec{r}) \equiv \textstyle\sum_{\mu,\nu=x}^{z} \epsilon_{\kappa\mu\nu} \, J_{q,\mu\nu}(\vec{r})$$ Spin-orbit

$$\tilde{\rho}_q(\vec{r}) \equiv \textstyle\sum_\sigma \kappa_{\vec{r}\sigma q \vec{r}\bar{\sigma} q} \, \sigma_z^{\bar{\sigma}\bar{\sigma}}$$ Pair

- Build scalar EDF from such densities, e.g. at $2^{nd}$ order in $\sigma_\nu$ and $\nabla$

# Empirical parameterizations of $\mathcal{E}[\rho,\kappa,\kappa^*]$ ; e.g. Skyrme or Gogny

## Local Skyrme EDF for even-even nuclei ground-state

- Universal form ($A \gtrsim 16$) but no universal parametrization

$$\mathcal{E}[\rho,\kappa,\kappa^*] = \sum_{qq'} \int d\vec{r} \Bigg[ C^{\rho\rho}_{qq'} \, \rho_q(\vec{r}) \, \rho_{q'}(\vec{r}) + C^{\rho\Delta\rho}_{qq'} \, \rho_q(\vec{r}) \, \Delta\rho_{q'}(\vec{r}) + C^{\rho\tau}_{qq'} \, \rho_q(\vec{r}) \, \tau_{q'}(\vec{r})$$

$$+ C^{\rho\nabla J}_{qq'} \, \rho_q(\vec{r}) \, \vec{\nabla}\cdot\vec{J}_{q'}(\vec{r}) + C^{JJc}_{qq'} \sum_{\mu,\nu=x}^{z} J_{q,\mu\nu}(\vec{r}) \, J_{q',\mu\nu}(\vec{r})$$

$$+ C^{JJt}_{qq'} \sum_{\mu,\nu=x}^{z} \Big[ J_{q,\mu\mu}(\vec{r}) \, J_{q',\nu\nu}(\vec{r}) + J_{q,\mu\nu}(\vec{r}) \, J_{q',\nu\mu}(\vec{r}) \Big] \Bigg]$$

$$+ \sum_{q} \int d\vec{r} \, C^{\tilde{\rho}\tilde{\rho}}_{qq} \, |\tilde{\rho}_q(\vec{r})|^2 + \text{additional terms involving gradients}$$

- Density-dependent couplings, i.e. $C^{ff'}_{qq'}$ may depend on $\vec{r}$ as well
- Fitted on INM OES and selection of finite nuclei data
- Usually derived from the density-dependent Skyrme+DDD "interaction"

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$$+ \sum_{q} \int d\vec{r}\, C^{\tilde{\rho}\tilde{\rho}}_{qq} |\tilde{\rho}_q(\vec{r})|^2 + \text{additional terms involving gradients}$$

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# Empirical parameterizations of $\mathcal{E}[\rho,\kappa,\kappa^*]$ ; e.g. Skyrme or Gogny

## Density-dependent Skyrme "force" for the particle-hole part

- Schematic effective vertex, i.e. a convenient intermediate to generate $\mathcal{E}^{\rho\rho^{1+\alpha}}$

$$
\begin{aligned}
v_{\text{cent}} &= t_0\,(1+x_0 P_\sigma)\,\delta(\vec{r}) \\
&+ \frac{1}{2}\,t_1\,(1+x_1 P_\sigma)\left[\delta(\vec{r})\,\overrightarrow{k}^2 + \overleftarrow{k'}^2\,\delta(\vec{r})\right] \\
&+ t_2\,(1+x_2 P_\sigma)\,\overleftarrow{k'}\cdot\delta(\vec{r})\,\overrightarrow{k} \\
&+ \frac{1}{6}\,t_3\,(1+x_3 P_\sigma)\,\rho_0^\alpha(\vec{r})\,\delta(\vec{r}) \\
v_{\text{ls}} &= iW_0\,(\vec{\sigma_1}+\vec{\sigma_2})\,\overleftarrow{k'}\wedge\delta(\vec{r})\,\overrightarrow{k} \\
v_{\text{tens}} &= \frac{t_e}{2}\left\{\left[3\,(\vec{\sigma}_1\cdot\overleftarrow{k'})\,(\vec{\sigma}_2\cdot\overleftarrow{k'}) - (\vec{\sigma}_1\cdot\vec{\sigma}_2)\,\overleftarrow{k'}^2\right]\delta(\vec{r})\right. \\
&\qquad \left. +\delta(\vec{r})\left[3\,(\vec{\sigma}_1\cdot\overrightarrow{k})\,(\vec{\sigma}_2\cdot\overrightarrow{k}) - (\vec{\sigma}_1\cdot\vec{\sigma}_2)\,\overrightarrow{k}^2\right]\right\} \\
&+ t_o\left\{3\,(\vec{\sigma}_1\cdot\overleftarrow{k'})\,\delta(\vec{r})\,(\vec{\sigma}_2\cdot\overrightarrow{k}) - (\vec{\sigma}_1\cdot\vec{\sigma}_2)\,\overleftarrow{k'}\cdot\delta(\vec{r})\,\overrightarrow{k}\right\}
\end{aligned}
$$

- Only $C^{\rho\rho}_{qq'}$ depends on the density

# Empirical parameterizations of $\mathcal{E}[\rho, \kappa, \kappa^*]$ ; e.g. Skyrme or Gogny

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## Density-dependent delta "interaction" for the particle-particle part

- Schematic effective vertex, i.e. a convenient intermediate to generate $\mathcal{E}^{\kappa\kappa}$

$$\tilde{v}_{\text{cent}} = \frac{1}{2}\,\tilde{t}_0 \left(1 - \eta\,\frac{\rho_0(\vec{r})}{\rho_{\text{sat}}}\right)(1 - P_\sigma)\,\delta(\vec{r})$$

- $C_{qq}^{\tilde{\rho}\tilde{\rho}}(\vec{r})$ is constant over the "Volume" ($\eta = 0$) or "Surface"-peaked ($\eta = 1$)
- Pairing correlations
  1. Are characterized by the dependence of the EDF on $\kappa/\tilde{\rho}$
  2. Are responsible for the superfluid nature of (most of the) nuclei
  3. Impact low-energy properties of finite nuclei and neutron stars
  4. Reflect (mostly) the strong NN attraction in the $^1S_0$ channel

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## Density-dependent delta "interaction" for the particle-particle part

- Schematic effective vertex, i.e. a convenient intermediate to generate $\mathcal{E}^{\kappa\kappa}$

## Energy density functional $\mathcal{E}[\rho, \kappa, \kappa^*]$

- Does NOT mimic a Hartree-Fock approximation in terms of NN+NNN
- Mocks up correlations BEYOND Hartree-Fock (see Lecture 3)
  1. Through rich (enough?) functional form
  2. Through fitting of parameters
- Not all correlations are easily resummed into $\mathcal{E}[\rho, \kappa, \kappa^*]$ itself
  1. Symmetry breaking captures important correlations
  2. Need for explicit configuration mixing = Multi-reference EDF method

# Single-particle field $h^q$

## $h^q$ from the Skyrme EDF

$$h_{ij}^q \equiv \frac{\delta \mathcal{E}}{\delta \rho_{ji}^q} = \int d\vec{r}\, \varphi_i^\dagger(\vec{r})\, h^q(\vec{r})\, \varphi_j(\vec{r})$$

where the local field takes the form

$$h_q(\vec{r}) \equiv -\nabla \cdot B_q(\vec{r}) \nabla + U_q(\vec{r}) - \frac{i}{2} \sum_{\mu,\nu=x}^{z} \left[ W_{q,\mu\nu}(\vec{r})\, \nabla_\mu + \nabla_\mu\, W_{q,\mu\nu}(\vec{r}) \right] \sigma_\nu$$

with multiplicative potentials defined as

$$U_q(\vec{r}) \equiv \frac{\delta \mathcal{E}}{\delta \rho_q(\vec{r})}$$

$$B_q(\vec{r}) \equiv \frac{\delta \mathcal{E}}{\delta \tau_q(\vec{r})}$$

$$W_{q,\mu\nu}(\vec{r}) \equiv \frac{\delta \mathcal{E}}{\delta J_{q,\mu\nu}(\vec{r})}$$

# Single-particle field $h^q$

## $h^q$ drives the correlated (!) s.p. motion

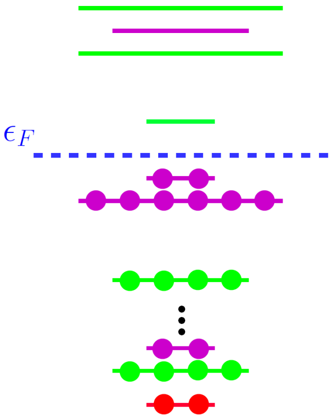
- $h^q$ provides the "shell structure"

$$h^q(\vec{r})\,\varphi_i(\vec{r}) \quad \equiv \quad \epsilon_i\,\varphi_i(\vec{r})$$

1. Separation energies
   - $\epsilon_p \approx \mathcal{E}_p^{N+1} - \mathcal{E}_0^N \approx E_p^{N+1} - E_0^N$
   - $\epsilon_h \approx \mathcal{E}_0^{N} - \mathcal{E}_h^{N-1} \approx E_0^{N} - E_h^{N-1}$
2. Excitation energies
   - $\epsilon_p - \epsilon_h \approx \mathcal{E}_{ph}^{N} - \mathcal{E}_0^N \approx E_{ph}^{N} - E_0^N$

- Keep in mind missing correlations

1. Symmetry breaking
   - Pairing via breaking of $N$
   - Quadrupole via breaking of $J^2$
2. Configuration mixing
   - Symmetry restorations
   - Dynamical part-vib coupling



# Pairing field $\Delta^q$

## $\Delta^q$ from the Skyrme EDF

$$\Delta^q_{ij} \quad \equiv \quad \frac{\delta \mathcal{E}}{\delta \kappa^{q\,*}_{ij}} = \int d\vec{r} \left[ \varphi^\dagger_i(\vec{r}q)\, \Delta_q(\vec{r})\, \varphi^*_j(\vec{r}q) - \varphi^\dagger_j(\vec{r}q)\, \Delta_q(\vec{r})\, \varphi^*_i(\vec{r}q) \right]$$

where the local field takes the form

$$\Delta_q(\vec{r}) \quad = \quad -\tilde{U}_q(\vec{r})\, i\sigma_y + \cdots$$

with multiplicative potentials defined as

$$\tilde{U}_q(\vec{r}) \quad \equiv \quad \frac{\delta \mathcal{E}}{\delta \tilde{\rho}^*_q(\vec{r})}$$

$$\vdots$$

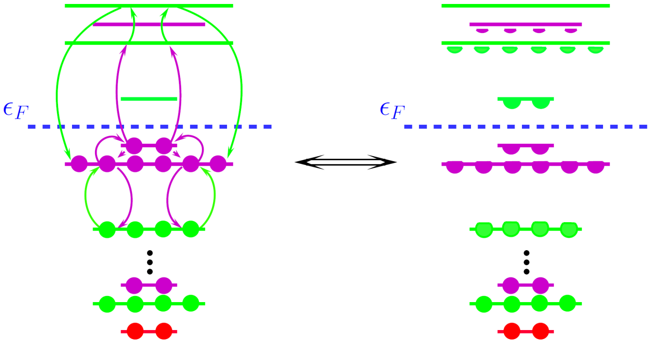
- UV divergence of local pairing EDF must be regularized/renormalized

# Pairing field $\Delta^q$

## $\Delta^q$ drives pair scattering

- Correlates nucleon pairs in time-reversal states
- Results in smoothed-out single-particle occupations (canonical basis)

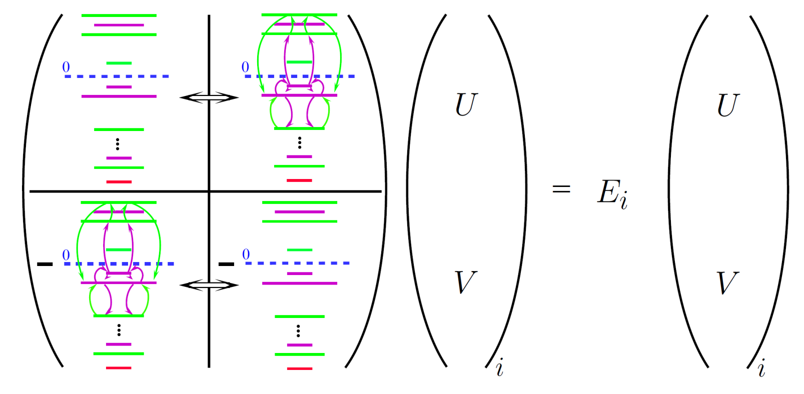
$$\rho_{ii} = v_i^2 = \frac{1}{2}\left[1 - \frac{\epsilon_i - \epsilon_F}{\sqrt{(\epsilon_i - \epsilon_F)^2 + \Delta_{i\bar{i}}^2}}\right]$$



# Hartree-Fock-Bogoliubov scheme

## Hartree-Fock-Bogoliubov eigenvalue problem

- Modified $v_i^2$ feedback onto $h^q$ which feedbacks onto pair scattering. . .




- Quasi-particle energy $E_i \approx \sqrt{(\epsilon_i - \epsilon_F)^2 + \Delta_{i\bar{i}}^2} \geq \Delta_F$

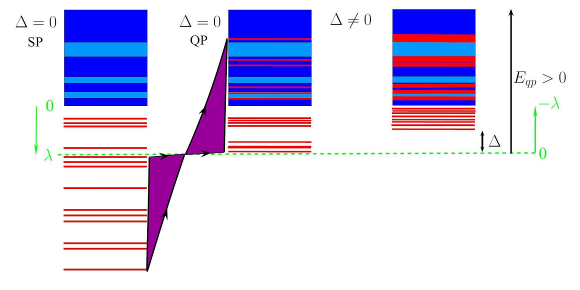
# Hartree-Fock-Bogoliubov scheme

## Hartree-Fock-Bogoliubov eigenvalue problem

- Pairing changes the nature of elementary excitations $|\Phi_{ij}\rangle = \beta_i^\dagger \beta_j^\dagger |\Phi\rangle$

$$\mathcal{E}_{ij}^{\langle N\rangle} - \mathcal{E}_0^{\langle N\rangle} = E_i + E_j \xrightarrow{\Delta=0} |\epsilon_p - \epsilon_F| + |\epsilon_h - \epsilon_F| = \epsilon_p - \epsilon_h$$

- Spectrum $E_i$ versus $|\epsilon_i - \epsilon_F|$




- Gap opens at low energy + mix of hole- and particle-like excitations

# Outline

# Performance of empirical EDFs (spherical HFB calculations)

## Performance of existing EDFs

- Tremendous over known nuclei
- Especially for bulk properties
- Role of symmetry breaking

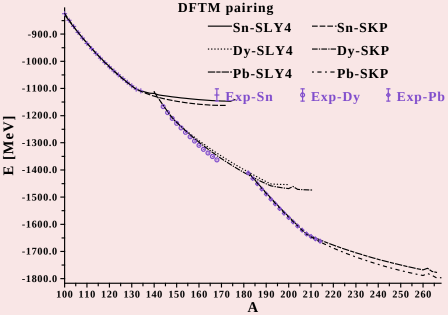
## "Asymptotic freedom"

- Into "the next major shell"
- For most observables
- Signals poor predictive power

## Spectroscopy

- The real challenge for the future...

## Binding energy in Sn, Dy and Pb isotopes




[J. Sadoudi, T. D., unpublished]

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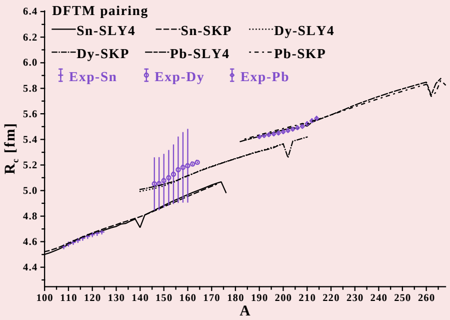
## Charge radius in Sn, Dy and Pb isotopes

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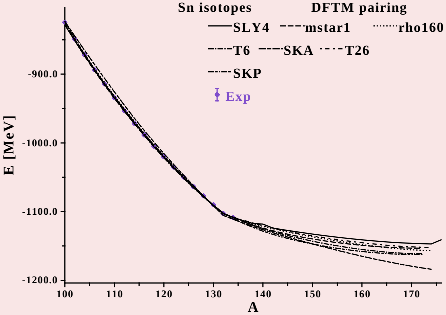


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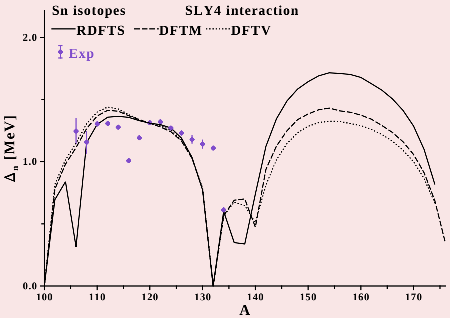
## Pairing gaps in Sn isotopes




[J. Sadoudi, T. D., unpublished]

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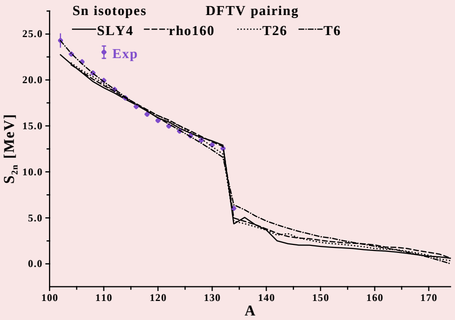
## Two-neutron sep. energy in Sn isotopes




[J. Sadoudi, T. D., unpublished]

# Performance of empirical EDFs

## Performance of existing EDFs

- Tremendous successes for known nuclei
- "Asymptotic freedom" as one enters "the next major shell"

## Crucial undergoing works

- Enrich the analytical structure of empirical functionals
  1. Tensor terms, e.g. [T. Lesinski et al., PRC76, 014312]
  2. Higher-order derivatives [B. G. Carlsson et al., PRC78, 044326]
  3. $\rho_n - \rho_p$ dependence to $C_{qq}^{\tilde{\rho}\tilde{\rho}}(\vec{r})$, e.g. [J. Margueron *et al.*, PRC77, 054309]
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- Improve fitting protocols = data, algorithm and post-analysis

## One can also propose a complementary approach. . .

- Data not always constrain unambiguously non-trivial characteristics of EDF
- Interesting not to rely entirely on trial-and-error and fitting data

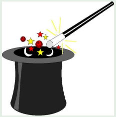
# Outline

# Constructing non-empirical EDFs for nuclei

**Long term objective**

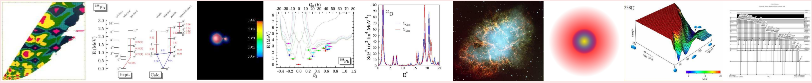
Build non-empirical EDF in place of existing models

**Empirical**



Predictive?

**Finite nuclei and extended nuclear matter**



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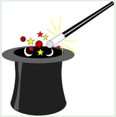
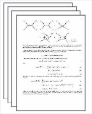


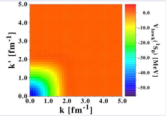
Predictive?

## Non-empirical

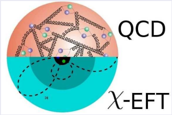


Predictive...

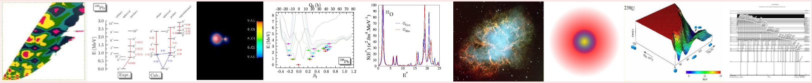
## Low-$k$ NN+NNN




## QCD / $\chi$-EFT




## Finite nuclei and extended nuclear matter



# Long term project and collaboration

**Design *non-empirical* Energy Density Functionals**

- Bridge with *ab-initio* many-body techniques
- Calculate properties of heavy/complex nuclei from NN+NNN
- Controlled calculations with theoretical error bars

| | |
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| NSCL | S. K. Bogner, B. Gebremariam |
| OSU | R. J. Furnstahl, L. Platter |
| ORNL | T. Lesinski |
| JULICH | A. Nogga |

# Outline

# Selected bibliography

P. Ring, P. Schuck,
*The nuclear many-body problem*, 1980, Springer-Verlag, Berlin

M. Bender, P.-H. Heenen, P.-G. Reinhard,
Rev. Mod. Phys. 75 (2003) 121