

# Functional approach for pairing with good Particle number

Denis Lacroix GANIL-Caen

> Coll: G. Hupin, M. Bender, Th. Duguet

# Outline of my talk



# Multi- Ref. (MR)-GCM

- Some recent discussion on symmetry breaking and Restoration in Energy Density Functional theory
  - Hamiltonian vs EDF
    - ⇒ Self-interaction problem
  - Density dependence of effective interaction ?

Can we interpret the MR-EDF as a functional theory?

- Proposition of a different strategy to break and restore symmetry in EDF : The Symmetry-Conserving EDF concept
- > Application to Particle number Restoration
- Examples of application of Projection before or After variation to light and medium mass nuclei
- DFT for small superconductors



#### Single Reference (SR)- $|\Psi\rangle = \int dQ f(Q) |\Phi(Q)\rangle$ Mean-Field Multi- Ref. (MR)-GCM $= \Pi \alpha_k |0\rangle$ $|\Phi\rangle$ 0 $|\Phi(Q_i)\rangle$ (Skyrme, Gogny) $\langle \Phi(Q) | \hat{H} | \Phi(Q) \rangle$ $\langle \Psi | \hat{H} | \Psi angle$ 8 -626 <sup>74</sup>Kr 712 pro--627Sly4-Bender, Bertsch, Heenen, PRL (2005) 6 $E_{exp} - E_{th} (MeV)$ **Mean-Field** -628 Energ 5E (MeV) (MeV)-629 4-630 8+ 3 Correlation E Energy -631 $\mathbf{2}$ -632 **Energy scale!** 1 1600 1000 -633 300 0 -12 -12 0.220 40 -0.4 -0.2 0.0 0.4 0.6 0.8 1.0 80 100120 140 160 60 Neutron number N $\beta_2$ Bender et al, PRC74 (2006)

#### **Configuration Mixing within Energy Density Functional**

# Breaking and restoring symmetries





#### Configuration mixing as a functional theory

The two-body Hamiltonian case: what is a functional of what?

$$H = \sum_{ij} t_{ij} a_i^{\dagger} a_j + \frac{1}{4} \sum_{ijkl} \bar{v}_{ijkl} a_i^{\dagger} a_j^{\dagger} a_l a_k$$

Mean-Field (with Pairing)

$$\begin{split} |\Phi_{0}\rangle &= \Pi\beta_{\alpha}^{\dagger}|-\rangle \\ \langle H\rangle &= \sum_{i} t_{ii}\rho_{ii} + \frac{1}{2}\sum_{i,j} \overline{v}_{ijij}\rho_{ii}\rho_{jj} + \frac{1}{4}\sum_{i,j} \overline{v}_{i\overline{\imath}j\overline{\jmath}}\kappa_{i\overline{\imath}}^{*}\kappa_{j\overline{\jmath}} \\ &= E_{SR}\left[\rho,\kappa,\kappa^{*}\right] \\ \Phi_{0} \to \left\{\rho,\kappa\right\} \to E_{SR} \end{split}$$

Projection

$$\begin{split} |\Psi_{\Omega}\rangle &= P^{\Omega}|\Phi_{0}\rangle \\ &= \int dQf(Q)|\Phi(Q)\rangle \\ E_{MR} &= \iint dQdQ'\mathcal{N}(Q,Q')E_{SR}(\rho^{QQ'},\kappa^{QQ'},\kappa^{*QQ'}) \\ \Phi_{0} &\to \{\rho^{QQ'},\kappa^{QQ'},\kappa^{*QQ'}\} \to E_{MR} \end{split} \qquad \Phi_{0} \to \Psi_{\Omega} \to \{\rho^{\Omega},R^{\Omega}\} \to E_{MR} \end{split}$$

$$|\Psi_{\Omega}\rangle = P^{\Omega}|\Phi_{0}\rangle$$

$$E_{MR} = \sum_{ij} t_{ij} \langle a_{i}^{\dagger} a_{j} \rangle_{\Omega}$$

$$+ \frac{1}{4} \sum_{ijkl} \bar{v}_{ijkl} \langle a_{i}^{\dagger} a_{j}^{\dagger} a_{l} a_{k} \rangle_{\Omega}$$

$$E_{MR} = \sum_{ij} t_{ij} \rho_{ij}^{\Omega} + \frac{1}{4} \sum_{ijkl} \bar{v}_{ijkl} R_{kl,ij}^{\Omega}$$

#### What about the EDF theory?

#### The particle number restoration case

Alternative formulation ?

#### For non-density dependent effective int.

 $|\Psi_N\rangle = P^N |\Phi_0\rangle$ 

Mean-Field (with Pairing)

 $P^N = \frac{1}{2\pi} \int_0^{2\pi} d\varphi \ e^{i\varphi(\hat{N}-N)}$ 

$$\begin{split} |\Psi_N\rangle &= P^N |\Phi_0\rangle \\ P^N &= \frac{1}{2\pi} \int_0^{2\pi} d\varphi \ e^{i\varphi(\hat{N}-N)} \end{split}$$

Mean-Field (with Pairing)

$$\begin{split} |\Phi_{0}\rangle &= \Pi \beta_{\alpha}^{\dagger} |-\rangle \\ \mathcal{E}_{SR}\left[\rho,\kappa,\kappa^{*}\right] &= \sum t_{ii}\rho_{ii} \\ &+ \frac{1}{2}\sum \overline{v}_{ijij}^{\rho\rho}\rho_{ii}\rho_{jj} + \frac{1}{4}\sum \overline{v}_{i\overline{\imath}j\overline{\jmath}}^{\kappa\kappa}\kappa_{i\overline{\imath}}\kappa_{j\overline{\jmath}} \\ \Phi_{0} &\to \{\rho,\kappa\} \to \mathcal{E}_{SR} \end{split}$$
Projection

$$\mathcal{E}_{N}[\Psi_{N}] \equiv \int_{0}^{2\pi} d\varphi \, \mathcal{E}_{SR}\left[\rho^{0\varphi}, \kappa^{0\varphi}, \kappa^{\varphi 0^{\star}}\right] \mathcal{N}_{N}(0,\varphi)$$

$$\Phi_0 \to \{\rho^{0\varphi}, \kappa^{0\varphi}, \kappa^{*0\varphi}\} \to \mathcal{E}_N$$

# What about the EDF theory

The particle number restoration case

Alternative formulation ?

For non-density dependent effective int. After regularization proposed in Lacroix, Duguet, Bender, PRC79 (2009)

$$\begin{aligned} \mathcal{E}_{N}[\Psi_{N}] &= \sum_{i} t_{ii} n_{i}^{N} \\ &+ \frac{1}{2} \sum_{i,j,j \neq \overline{\imath}} \overline{v}_{ijij}^{\rho\rho} R_{ijij}^{N} \\ &+ \frac{1}{4} \sum_{i \neq j,j \neq \overline{\imath}} \overline{v}_{i\overline{\imath}j\overline{\jmath}}^{\kappa\kappa} R_{j\overline{\jmath}i\overline{\imath}}^{N} \\ &+ \frac{1}{2} \sum_{i} \overline{v}_{i\overline{\imath}i\overline{\imath}}^{\rho\rho} (n_{i}^{N} n_{i}^{N} - \delta n_{i} \delta n_{i}) \\ &+ \frac{1}{2} \sum_{i} \overline{v}_{i\overline{\imath}i\overline{\imath}}^{\kappa\kappa} \left[ n_{i}^{N} (1 - n_{i}^{N}) + \delta n_{i} \delta n_{i} \right] , \\ &\delta n_{i} = n_{i}^{N} - n_{i}^{0} \\ &\Psi_{N} \end{aligned}$$

# What about the EDF theory



#### Discussion

Direct formulation:

 $\Psi_N \to \{\rho^N, R^N\} \to \mathcal{E}_{SC}(\rho^N, R^N)$ 

Advantages

- the functional is automatically symmetry conserving.
- It is equivalent to MR-EDF for non density dependent term
- It is a natural extension of SR-EDF



It is free of jumps/divergence

The Symmetry Conserving EDF



It could be extended to dens. dependent interaction  $\overline{v}^{\rho\rho}[\rho] \Longrightarrow \overline{v}^{\rho\rho}[\rho^N], \ \overline{v}^{\kappa\kappa}[\rho] \Longrightarrow \overline{v}^{\kappa\kappa}[\rho^N]$ 

#### Variation After Projection: the projected BCS case

 $\Psi_N \to \{\rho^N, R^N\} \to \mathcal{E}_{SC}(\rho^N, R^N)$ 

$$\mathcal{E}_{N}[\Psi_{N}] = \sum_{i} t_{ii} n_{i}^{N} + \frac{1}{2} \sum_{i,j,j\neq\bar{\imath}} \overline{v}_{ijij}^{\rho\rho} R_{ijij}^{N} + \frac{1}{4} \sum_{i\neq j,j\neq\bar{\imath}} \overline{v}_{i\bar{\imath}j\bar{\jmath}}^{\kappa\kappa} R_{j\bar{\jmath}i\bar{\imath}}^{N} + \frac{1}{2} \sum_{i} \overline{v}_{i\bar{\imath}i\bar{\imath}\bar{\imath}}^{\rho\rho} n_{i}^{N} n_{i}^{N} + \frac{1}{2} \sum_{i} \overline{v}_{i\bar{\imath}i\bar{\imath}\bar{\imath}}^{\kappa\kappa} n_{i}^{N} (1 - n_{i}^{N})$$

Trial state:

Functional:

$$|\Psi_N\rangle = P^N \Pi (u_i + v_i a_i^{\dagger} a_{\overline{i}}^{\dagger}) |-\rangle$$

Minimization:

$$\frac{\partial \mathcal{E}_N}{\partial v_i^2} = 0 \qquad \frac{\partial \mathcal{E}_N}{\partial \varphi_i^*(r)} = 0$$

L

Sheik, Ring, NPA665 (2000), Dietrich et al, PRB135 (1964)

Application:

Occupation Probability (BCS case)-ev8 code



# Variation After Projection: the projected BCS case



**Density Matrix Functional Theory** 

#### **Occupation-number based energy functionals**

Lieb (1983), Papenbrock, Bhattacharyya, PRC75 (2007) ; Bertolli, Papenbrock, PRC78 (2008) ; Lacroix, PRC79 (2009)

$$F(\{n_j\}) = E - \sum_{k=1}^{M} n_k \varepsilon_k \text{ with } n_k \equiv \frac{\partial E}{\partial \varepsilon_k}$$

BCS, RPA, NLO...

•Richardson model
•2- and 3-level Lipkin
•Some motivation for the Duflo-Zuker mass formula

#### **Density Matrix Functional Theory (DMFT) for electronic systems**

Gilbert (1975). Klooster, http://theochem.chem.rug.nl/publications/Abstracts.html#587.



# **Functional Theory for Pairing with particle number conservation** BCS *vs* Projected BCS state

Test on a model case : Pairing Hamiltonian

# **Functional Theory for Pairing with particle number conservation** BCS *vs* Projected BCS state

Illustration: Richardson Hamiltonian

$$E \rightarrow \mathcal{E}(n_{i}, C_{ij}) = \sum_{i} \varepsilon_{i} n_{i} + -\frac{g}{2} \sum_{i,j} C_{ij} \quad \text{with} \quad n_{i} = \frac{\langle \Phi | a_{i}^{\dagger} a_{i} | \Phi \rangle}{\langle \Phi | \Phi \rangle}, \quad C_{ij} = \frac{\langle \Phi | a_{i}^{\dagger} a_{i}^{\dagger} a_{j} a_{j} | \Phi \rangle}{\langle \Phi | \Phi \rangle}$$

$$BCS$$

$$|BCS\rangle \propto \prod_{i} (1 + x_{i} a_{i}^{\dagger} a_{i}^{\dagger})| - \rangle$$

$$x_{i} = (v_{i}/u_{i})$$

$$n_{i} = \frac{|x_{i}|^{2}}{(|x_{i}|^{2} + 1)}$$

$$C_{ij} = \frac{x_{i}^{*} x_{j}}{(|x_{i}|^{2} + 1)(|x_{j}|^{2} + 1)}$$

$$\mathcal{E}(\{x_{i}\})$$

$$n_{i} = N|x_{i}|^{2} \frac{\sum_{(i_{1}, \cdots i_{N}) \neq (i_{N})}^{\neq} |x_{i_{1}}|^{2} \cdots |x_{i_{N}}|^{2}}{\sum_{(i_{1}, \cdots i_{N}) \neq (i_{N})}^{\neq} |x_{i_{1}}|^{2} \cdots |x_{i_{N}}|^{2}}$$

$$C_{ij} = Nx_{i}^{*} x_{j} \frac{\sum_{(i_{1}, \cdots i_{N}) \neq (i_{N})}^{\neq} |x_{i_{1}}|^{2} \cdots |x_{i_{N}}|^{2}}{\sum_{(i_{1}, \cdots i_{N}) \mid}^{\neq} |x_{i_{1}}|^{2} \cdots |x_{i_{N}}|^{2}}$$

$$\mathcal{E}(\{n_{i}\})$$

### **Explicit Functional of occupation numbers for Pairing**

$$n_{i} = N|x_{i}|^{2} \frac{\sum_{(i_{1},\dots,i_{N-1})\neq(i)}^{\neq} |x_{i_{1}}|^{2} \dots |x_{i_{N-1}}|^{2}}{\sum_{(i_{1},\dots,i_{N})}^{\neq} |x_{i_{1}}|^{2} \dots |x_{i_{N}}|^{2}} \longrightarrow x_{i} = \mathcal{F}(n_{i})$$

#### A new systematic 1/N expansion beyond BCS:



All contributions can be approximately summed to give:

$$|x_i|^2 = \left(\frac{n_i}{1-n_i}\right) [a_0 + a_1 n_i + \cdots]$$

BCS

$$a_1 = -\frac{1}{N} \frac{1 - s_2^N}{1 - s_2}$$

$$a_0 = 1 - (s_2 - s_3) \frac{\partial a_1}{\partial s_2}$$



with

Lacroix and Hupin, PRB82 (2010), Hupin, Lacroix, PRC83 (2011)

 $s_2 = \frac{1}{N} \sum_{i} n_i^2$   $s_3 = \frac{1}{N} \sum_{i} n_i^3$ 



#### **Summary**



In some cases, the MR-EDF can be interpreted as a functional Of the one- and two-body density of the projected state

 $\Psi_N \to \{\rho^N, R^N\} \to \mathcal{E}_{SC}(\rho^N, R^N)$ 

This provides a different way to perform projection in EDF

- No pathologies
- Consistent with SR-EDF
- Directly applicable (PAV and VAP)



We further simplify the problem using DMFT

$$\Psi_N \to \{n_i^N, \varphi_i\} \to \mathcal{E}_{MR}$$

**Outlooks** 

Systematic Nuclear Structure study with Variation After projection

Time-Dependent EDF with pairing

Thermodynamics of systems with pairing

# **Explicit Functional of occupation numbers for Pairing**

