Pairing schemes for HFB calculations: Formal aspects

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Effect of pairing on structure properties

I. Individual excitation spectra:

*Gap for even-even nuclei ⇒ a (quite) direct measure of the gap

II. Odd-even mass staggering (OES)

III. Collective excitations ⇒ less direct measure but sensitive to the spatial structure of the force

*Rotational: $\nearrow \mathcal{J}^{(2)} = -\frac{\partial^2 \mathcal{E}^\omega}{\partial^2 \omega}$ with ω

*Vibrational states: low-lying states → especially in exotic nuclei

*Shape isomers: from intruders

IV. Width of deep-hole states

V. Matter density (reduces halos)

VI. Pair transfer

VII. Glitches in the inner crust of neutron stars

VIII. Cooling of neutron stars: emission processes and heat diffusion

Framework using gauge invariance symmetry breaking

I. **Many-body perturbation theory** written in terms of the bare nucleon-nucleon force:

*Green-function's formalism
Galitskii, Migdal, Gorkov using non-time-ordered diagrams

*Goldstone formalism
Bogolyubov, Mehta, Henley and Wilets using time-ordered diagrams

II. **Density Functional Theory** a la Hohenberg-Kohn/Kohn-Sham:

*Fully non-local theory **(well-behaved)**
Oliveira et al. (1988) for High-T_c superconductors

*Local theory **(including microscopic regularization schemes)**
Bruun et al. (1999) for trapped ultracold fermionic atoms
Bulgac and Yu (2002) for finite nuclei

III. **Variational-type** HFB calculations:

*Fully non-local theory **(regularized through the finite range)**
Déchargé and Gogny (1981) for finite nuclei

*Local theory **(including phenomenological regularization schemes)**
Dobaczewski et al. (1984) for finite nuclei

Main ingredients for pairing

I. The global amount of pairing (in the ground-state as a start) depends on:

*The number of particles outside a closed-shell

*The density of s.p. states around the Fermi surface $\Leftarrow m^\star$, level of approx

*The proximity of the s.p. continuum

II. Pairing properties and their trends (toward drip-lines for instance) depend on:

*The characteristics of the effective pairing force/functional used:

$\longrightarrow$ isoscalar and isovector density-dependence

$\longrightarrow$ range? or regularization (+ gradient corrections)?

*The level of approximation one is working at:

$\longrightarrow$ mean-field = static pairing

$\longrightarrow$ beyond = coupling to vibrations and dynamical pairing

Influence on low-energy nuclear structure?

Phenomeno. zero-range effective forces/local functionals

I. Generalities

*Underlying mean-field usually generated by a Skyrme functional/Gogny force

*Pairing in the $^1S_0$ channel for now (n-n and p-p)

*Only phenomenological schemes have been used in finite nuclei so far

*No attempt to construct non-empirical Kohn-Sham functional

II. Standard *Density Dependent Delta Interaction* (DDDI)/local functional quadratic in $\tilde{\rho}^q$:

$$E^{p-p} = \frac{1}{4} \sum_q \int d\vec{r}\, t'_0\, f_{DDDI}(\vec{r})\, \tilde{\rho}^{q\,2}(\vec{r}) \qquad \text{with} \qquad f_{DDDI}(\vec{r}) = \left[1 - \eta \left(\frac{\rho_0(\vec{r})}{\rho_{sat}}\right)^{\gamma}\right]$$

*$\tilde{\rho}^q(\vec{r})$ is the local/spin-singlet part of the pairing tensor

*$\rho_0(\vec{r})$ is the local/scalar/isoscalar part of the normal density matrix

*$\eta = 0 \leftrightarrow$ *Volume (V)*

$1/2 \leftrightarrow$ *Mixed (M)*

$1 \leftrightarrow$ *Surface (S)*

*The smaller γ, the stronger the interaction at low density

*Surface enhanced interaction was motivated by ab-initio calculations of $\Delta_{k_F}(k_F)$ in INM

Phenomeno. regularization schemes

I. Mainly used phenomenological regularization schemes are

Name	Basis	Scheme	Regularized Quantity
ULB	Can.	$\lambda - \epsilon_{cut} \leq \epsilon_{can} \leq \lambda + \epsilon_{cut}$	$\tilde{\rho}^q(\vec{r}) \Rightarrow \Delta$ and E^{p-p}
DFT	Q. P.	$E_{qp} \leq E_{cut}$	$\tilde{\rho}^q(\vec{r}) \Rightarrow \Delta$ and E^{p-p}

*"*ULB*" with $\epsilon_{cut} = 5 MeV$

$$\tilde{\rho}^q_{cut}(\vec{r}) = 2 \sum_{i>0,\,\sigma} g_i^{ULB} \, |\varphi_i(\vec{r}\sigma q)|^2 \, u_{iq} \, v_{\bar{i}q} \qquad \text{with} \qquad g_i^{ULB} = \frac{1}{1 + e^{(\epsilon_{iq} - \lambda^q - \epsilon_{cut})/\Delta\epsilon}} \, \frac{1}{1 + e^{-(\epsilon_{iq} - \lambda^q - \epsilon_{cut})/\Delta\epsilon}}$$

*"*DFT*" with $E_{cut} = 60 MeV$

$$\tilde{\rho}^q_{cut}(\vec{r}) = - \sum_{0<E_i,\,\sigma} g_i^{DFT} \, \Psi_2(E_i, \vec{r}\sigma q) \, \Psi_1^*(E_i, \vec{r}\sigma q) \qquad \text{with} \qquad g_i^{DFT} = \frac{1}{1 + e^{(E_i - E_{cut})/\Delta\epsilon}}$$

II. The local pairing gap

$$\Delta^q(\vec{r}) = \frac{1}{2} \, t_0' \, f_{DDDI}(\vec{r}) \, \tilde{\rho}^q_{cut}(\vec{r})$$

III. t_0' is adjusted accordingly using one's preferred recipe . . .

Current situation

I. Physics issues

*Existing schemes are successful over the known mass table

*Limited predictive power for unknown regions (very different predictions)

II. We need to

*Improve on usual DDDI $\Rightarrow$ Regularization and (isovector) density-dependence

*Understand whether resolving the finite range of the force is necessary

*Understand bare force's contribution to pairing in finite nuclei (Barranco et al., (2004))

*Understand what is needed beyond?

III. Technical issues

*Simple forms required to perform extensive 3D HFB calculations of finite nuclei

*Even more critical when going beyond the mean-field

Microscopic regularization in the DFT context = *"RDFT"*

I. Infinite matter : ultraviolet divergence of the pairing density *Bulgac and Yu (2002)*

$$\lim_{\vec{r}_1 \to \vec{r}_2} \tilde{\rho}^q(\vec{r}_1, \vec{r}_2) = \tilde{\rho}^q_{reg}(\vec{r}_2) + \lim_{\vec{r}_1 \to \vec{r}_2} \frac{m}{4\pi\hbar^2} \frac{\Delta \exp(ik_F|\vec{r}_1 - \vec{r}_2|)}{|\vec{r}_1 - \vec{r}_2|} = +\infty$$

$\Rightarrow$ throw away the divergent part $m/2\pi\hbar^2|\vec{r}_1 - \vec{r}_2|$ in the limit $\vec{r}_1 - \vec{r}_2 \to 0$

II. Finite nuclei: Thomas-Fermi approximation of the HF propagator $= k_F \to k_F(\vec{r})$

$$\tilde{\rho}^q_{cut}(\vec{r}) = - \sum_{0<E_i<E_{cut},\,\sigma} \Psi_2(E_i, \vec{r}\sigma q)\, \Psi_1^*(E_i, \vec{r}\sigma q),$$

$$\Delta^q(\vec{r}) = \frac{1}{2} t_0'\, f_{DDDI}(\vec{r})\, \tilde{\rho}_{reg}(\vec{r}) = \frac{1}{2} t_0^{eff\,\prime}(\vec{r})\, f_{DDDI}(\vec{r})\, \tilde{\rho}_{cut}(\vec{r})$$

$$\frac{1}{t_0^{eff\,\prime}(\vec{r})} = \frac{1}{t_0'} - \frac{m k_c(\vec{r})}{2\pi^2\hbar^2} \left[1 - \frac{k_F(\vec{r})}{2k_c(\vec{r})} \ln \frac{k_c(\vec{r}) + k_F(\vec{r})}{k_c(\vec{r}) - k_F(\vec{r})}\right] = \text{Regulator in coordinate space}$$

with

$$\lambda^q \equiv \frac{\hbar^2 k_F^2(\vec{r})}{2m} + U(\vec{r}) \qquad \text{and} \qquad E_{cut} \equiv \frac{\hbar^2 k_c^2(\vec{r})}{2m} + U(\vec{r}) - \lambda^q$$

III. Comments

*One parameter less theory; systematic principle behind regularization method
*One is still left with constructing the functional for finite nuclei

A complementary approach : MBPT + bare NN force

Step by step construction of the functional (a priori non-local)

I. First step = **mean-field** picture = lowest-order in terms of **IRREDUCIBLE vertices**

Particle-hole:

In-medium two-body matrix ($G/T/V_{lowk}$ at 2^{nd} order)

Two-body scattering in the medium

Particle-particle:

BARE INTERACTION

Two-body bound state in the medium

$\Longleftrightarrow$ HFB = **Independent pairs approximation**

II. Beyond lowest order

*Screening effects due to spin and density fluctuations (dressed vertex and self-energy)
Shen et al. (2005); Terasaki et al. (2001)

*We want to understand that in the context of GCM/Projection

III. For now, the lowest order...

*Understand systematically the contribution of the bare force to pairing in finite nuclei
*Structure effects in exotic nuclei
*Setting up an approximate local functional containing (most of) this physics

Bare NN force in the $^1S_0$ channel

I. Realistic NN forces in their full glory are too involved

II. Impossible to use in systematic calculations of heavy nuclei

III. A solution T. D., PRC 69 (2004)

$$\langle \vec{k}_1 \vec{k}_2 \,|\, V_{sep} \,|\, \vec{k}_3 \vec{k}_4 \rangle \approx \lambda \; v(k)\; v(k')\; (2\pi)^3 \, \delta(\vec{P} - \vec{P}\,') \quad \text{with} \quad v(k) = e^{-\alpha^2 k^2}$$

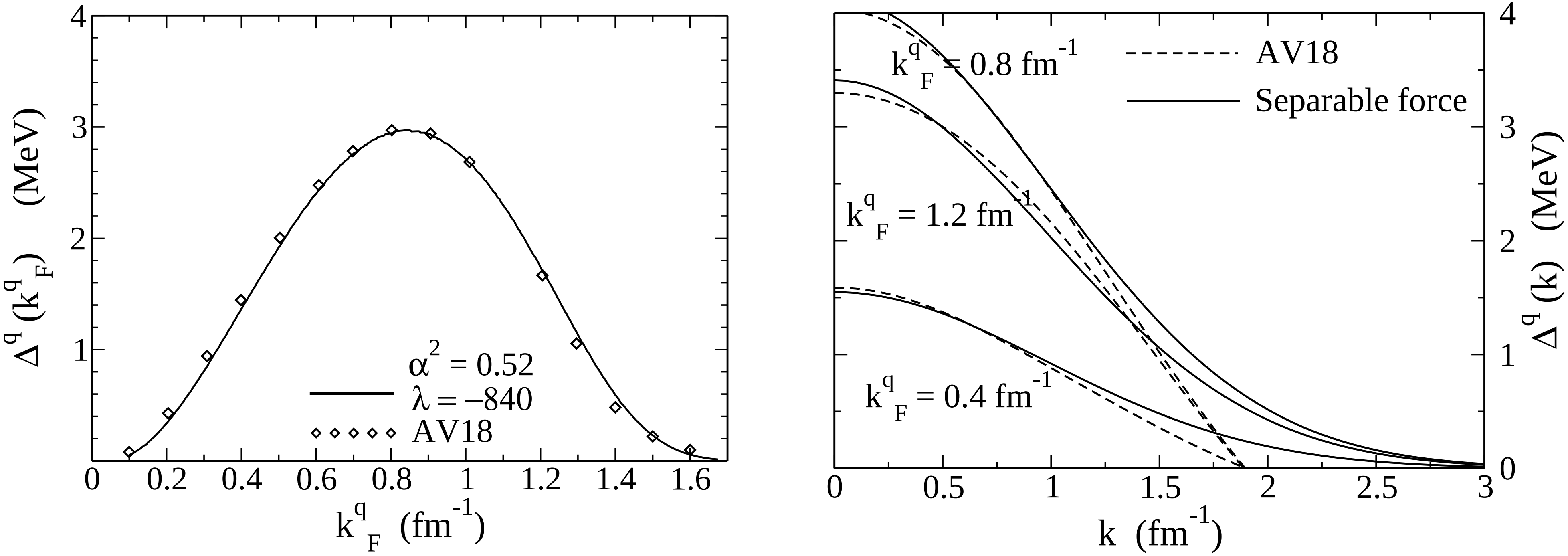
Very well justified at low energy (virtual di-neutron in the vacuum around 0 energy)

IV. Fit (using predictions from AV18 NN interaction, Wiringa *et al.* (1995))

*Phase shifts $\delta^{^1S_0}(k)$ from NN scattering

*Pairing gap from realistic NN interaction in infinite matter

III. Results in infinite matter (no self-energy at this point: $\epsilon(k) = k^2/2m$)



*The separable force is able to reproduce fine pairing properties:

$\Delta^q(k_F)$ up to the gap closure AND $\Delta^q(k)$ $\forall\, k$

*The Gogny force is close to V_{sep} and $V_{low\,k}$ (stronger though)

IV. Self-consistent HFB calculations of finite nuclei in coordinate space: V_{sep} is still untractable

V. Link to density-dependent zero-range interactions: not obvious

VI. Exact reformulation of the pairing problem in terms of an effective force

Combine $\Delta^q_{i\bar{\imath}} = -\sum_j \langle\, i\, \bar{\imath} \,|\, V_{sep} \,|\, j\, \bar{\jmath} \,\rangle\, u_{jq}\, v_{jq}$

with $\langle\, i\, j \,|\, \mathcal{R}(s) \,|\, k\, l \,\rangle = \langle\, i\, j \,|\, V_{sep} \,|\, k\, l \,\rangle + \sum_{mn} \langle\, i\, j \,|\, \mathcal{R}(s) \,|\, m\, n \,\rangle\; F^{\mathcal{R}}_{mn}(s)\; \langle\, m\, n \,|\, V_{sep} \,|\, k\, l \,\rangle$

VII. Freedom in the choice of $F^{\mathcal{R}}_{mn}(s) \Rightarrow$ sums p-p and h-h ladders in the **superfluid**

$$F^{\mathcal{D}/\mathcal{T}}_{mn}(0) = -\frac{(1-v^2_{mq})\,(1-v^2_{nq})}{E_{mq}+E_{nq}} \pm \frac{v^2_{mq}\, v^2_{nq}}{E_{mq}+E_{nq}}$$

$$\Delta^q_{i\bar{\imath}} = -\sum_j \langle\, i\, \bar{\imath} \,|\, \mathcal{D}(0) \,|\, j\, \bar{\jmath} \,\rangle\, 2\, v^2_{jq}\;\; u_{jq}\, v_{jq}$$

$$\Delta^q_{i\bar{\imath}} = -\sum_j \langle\, i\, \bar{\imath} \,|\, \mathcal{T}(0) \,|\, j\, \bar{\jmath} \,\rangle\, 2\,(1-v^2_{jq})\, v^2_{jq}\;\; u_{jq}\, v_{jq}$$

VIII. Effective pairing interactions:

$$\langle i\,\bar{\imath}\,|\,V_q^{eff\,\mathcal{D}}\,|\,j\,\bar{\jmath}\rangle \equiv \langle i\,\bar{\imath}\,|\,\mathcal{D}(0)\,|\,j\,\bar{\jmath}\rangle\,2\,v_{jq}^2$$

$$\langle i\,\bar{\imath}\,|\,V_q^{eff\,\mathcal{T}}\,|\,j\,\bar{\jmath}\rangle \equiv \langle i\,\bar{\imath}\,|\,\mathcal{T}(0)\,|\,j\,\bar{\jmath}\rangle\,2\,(1-v_{jq}^2)\,v_{jq}^2$$

*Both are exact and equivalent (between themselves and to the starting point = bare force)

*Of course, not true anymore if approximations are made on $\mathcal{D}(0)/\mathcal{T}(0)$

*Resum high-E virtual excitations → treat non-linear pair scatterings through the gap equation

*Natural **cut-off** in the gap equation = regularization scheme in the medium

Asymmetric version around λ^q: $2\,v_{jq}^2$ $\Longrightarrow$ **together with** $\mathcal{D}(0)$

Symmetric version around λ^q: $2\,(1-v_{jq}^2)\,v_{jq}^2$ $\Longrightarrow$ **together with** $\mathcal{T}(0)$

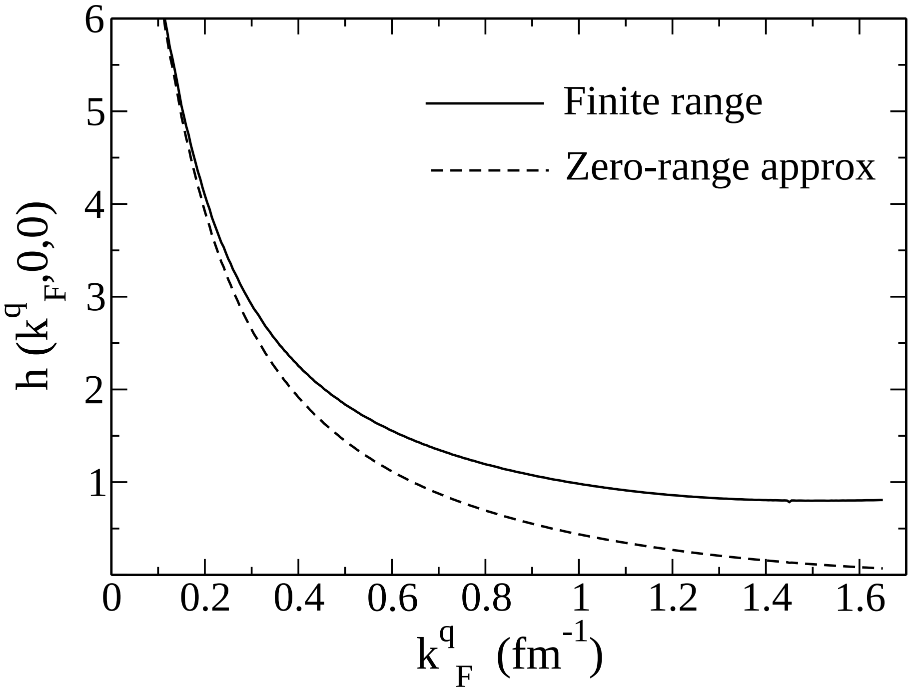
*$V_q^{eff\,\mathcal{D}/\mathcal{T}}$ depends on the medium ⇒ isoscalar and isovector density dependences

Appropriate scheme to study range (and regularization) vs density-dependence

$V^{eff\,\mathcal{D}}$ effective interaction in infinite matter

I. Form $\quad \langle \vec{k}\,|\,\mathcal{D}[k_F^q](0)\,|\,\vec{k}\,'\rangle = \lambda\; f(k_F^q)\; v(k)\; v(P/\sqrt{2})\; v(k') = \lambda\; f(k_F^q)\; \exp\left[-\alpha^2\,\left(k^2 + P^2/2 + k'^{\,2}\right)\right]$

II. Density dependence: $f_{(Z)FR}(k_F^q)$



*$f_{(Z)FR}(k_F^q) \approx A_{(Z)FR} + B_{(Z)FR} \ln k_F^q + C_{(Z)FR}\,(\ln k_F^q)^2$

*Strong enhancement at low-density $\Longleftrightarrow$ virtual state in the vacuum

*Zero-range approx: surf/vol $\nearrow$ = **pure density effect renormalizing the finite range**

*Finite range can be kept for calculations of finite nuclei (gradient corrections to all orders)

HFB calculations in coordinate space

I. The force is finite-ranged, non-local and density-dependent:

$$\langle \vec{r}_1 \, \vec{r}_2 \, | \, \mathcal{D}_q(0) \, | \, \vec{r}_3 \, \vec{r}_4 \, \rangle = \frac{\lambda}{(2\pi)^6 \alpha^{12}} \int d\vec{r} \; f_{FR}(\vec{r}) \; e^{-\sum_{i=1}^{4} |\vec{r}-\vec{r}_i|^2/2\alpha^2} \qquad \text{with} \qquad f_{FR}(\vec{r}) \equiv f_{FR}(k_F^q(\vec{r}))$$

but

$$\begin{aligned}
\hat{\tilde{\rho}}^q_{reg}(\vec{r}) &= 2 \sum_{i>0,\,\sigma} 2\, v_{iq}^2 \, |\hat{\varphi}_i(\vec{r}\sigma q)|^2 \, u_{iq} \, v_{\bar{i}q} \\
\hat{\Delta}^q_{reg}(\vec{r}) &= \frac{1}{2} \lambda \, f_{FR}(\vec{r}) \, \hat{\tilde{\rho}}^q_{reg}(\vec{r}) \\
E^{p-p} &= \frac{1}{2} \sum_q \int d\vec{r} \, \hat{\Delta}^q_{reg}(\vec{r}) \, \hat{\tilde{\rho}}^{\,q} \, (\vec{r})
\end{aligned}$$

with $\bar{\varphi}_i(\vec{r}\sigma q) = \frac{1}{(\sqrt{2\pi}\,\alpha)^3} \int d\vec{r}\,' \, e^{-|\vec{r}-\vec{r}\,'|^2/2\alpha^2} \, \varphi_i(\vec{r}\,'\sigma q)$

*Same form as for a zero-range force + convoluted canonical w.f.

*CPU / systematic 3D HFB calculations in coordinate space through 2-basis method are tractable

*Requires only trivial modifications of existing codes

Regularization scheme: comparison between *RDFT* and $"2v_{iq}^2"$

*Same idea of taking care of the ultraviolet divergence in the medium

*Use very different technics

*Are expressed in different basis: coordinate basis vs canonical basis

***However, they regularize the pairing problem in the same way**

$$\frac{1}{|t'_0|} = \int_0^{k_c} dk \frac{k^2}{4\pi^2} \left[\frac{1}{\sqrt{[\epsilon(k)-\lambda]^2 + \Delta^2}} - h(k) \right] \underset{k_c \to \infty}{\longrightarrow} \text{finite}$$

-Asymmetric RDFT and $2v_k^2$: $\left[\frac{1}{\sqrt{[\epsilon(k)-\lambda]^2+\Delta^2}} - h(k) \right] \underset{\epsilon_k \to +\infty}{\longrightarrow} \frac{\Delta^2}{2(\epsilon_k-\lambda)^3}$

-Symmetric RDFT and $2(1-v_k^2)v_k^2$: $\left[\frac{1}{\epsilon(k)-\lambda]^2+\Delta^2} - h(k) \right] \underset{\epsilon_k \to \pm\infty}{\longrightarrow} \frac{\Delta^2}{2|\epsilon_k-\lambda|^3}$

Regularization scheme: does it impact the physics?

I. Ex: **DFT** and **RDFT** only differs through the **regularization method**

$\Rightarrow$ comparison through 1D HFB calculations of semi-magic nuclei

$\Rightarrow$ SLy5 Skyrme parametrization in the p-h channel

$\Rightarrow$ f_{DDDI} with $\gamma = 1$ and $\eta = 1/2$ (very moderately enhanced at low dens)

Masses, S_{2N}, gaps, $\delta\langle r^2\rangle$, $\Delta(\vec{r})$ of spherical nuclei are almost identical

II. **BUT**: strongly rising intensity at low dens derived in the present work from NN force

$\Rightarrow$ Crucial to use a microscopic regularization scheme

$\Rightarrow$ Crucial to derive the microscopic cut-off and the density dependence accordingly

$\Rightarrow$ **K. Bennaceur's talk**

Summary

I. Microscopic pairing interaction in 3D HFB calculations in coordinate space

*Possible to handle the bare NN force through a recast of the pairing problem

*Finite range and non local

*Isoscalar and isovector density dependences as well as low density regime

*Confirmation of refine phenomenological study in favor of *Mixed* DDDI (Doba et al. (2001))

Perspectives

I. Extensive study T. D., K. Bennaceur and P. Bonche (2005) in preparation

*Convergence properties of different methods

*Detailed discussion of regularization schemes

*S_N and S_{2N} (drip-lines), Odd-even mass differences, PES, moment of inertia (cf. E_{pair})

*Systematic bare force's contribution to pairing in finite nuclei

*Spatial di-neutron correlations (cf. Matsuo et al. (2004)) : FR vs ZFR

*Individual excitations: FR vs ZFR

II. Near future

*Beyond mean-field (Projection + GCM methods): FR vs ZFR (with M. Bender)

*New Skyrme force adjusted with FR; mass tables (with T. Lesinski and K. Bennaceur)

*Systems probing the strong pairing force at low density (with B. Avez and V. Rotival)

*Coulomb for proton-proton pairing : DME treatment (with K. Bennaceur)

II. Future

*Effect of the three-body force on pairing properties

*Correction to the pairing vertex in GCM and Projection methods (with V. Rotival)