Neutron-proton pairing in nuclear density functional theory

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NSCL Theory Seminar

- Introduction to neutron-proton pairing
- Neutron-proton pairing in nuclear density functional theory

isobaric analogue states and isovector pairing

ground state neutron-proton pair condensation in N=Z nuclei

Neutron-proton pairing beyond nuclear DFT

double-beta decay nuclear matrix element and isoscalar pairing

□ Summary

Collective correlations

two levels of many-body correlation (in the terminology of mean field theory): residual correlation and condensation

residual correlation: no effect in the mean field level (beyond-mean-field effect)

condensation: structural change in the mean field

two main collective correlations in nuclei: pairing and multipole force

| force | residual correlation | condensation |
|------------------|---|------------------------|
| pairing force | pairing vibration of normal system | superconductivity |
| quadrupole force | quadrupole surface oscillation of spherical nucleus | quadrupole deformation |

Nucleonic pairing

pairing interaction

two nucleons in a time-reversed pair of orbits get additional binding

pairing relevant phenomena (condensation)

- one-neutron/proton separation energy $S_n(N,Z) = B(N,Z) - B(N-1,Z)$ $S_{p}(N,Z) = B(N,Z) - B(N,Z-1)$
- rotational moment of inertia
- two-nucleon transfer cross section
- level densities (even and odd systems)
- two-nucleon separation energy: NH and Nazarewicz (2016)

like-particle pairing (nn and pp) condensation exists everywhere in open-shell nuclei

pairing relevant phenomena (residual correlation)





Sn

18 16

14



Neutron-proton pairing

Nuclear force has (approximate) isospin symmetry nucleon: isospin t=1/2 (neutron $t_z=1/2$, proton $t_z=-1/2$)

many experimental evidence for nn ($T_z=1$) and pp($T_z=-1$) pairing condensation

Nucleon pairing for L=0 (space-symmetric) pair

Isovector (T=1, S=0) pairings: isospin symmetric, spin antisymmetric



Isoscalar (T=0, S=1) pairings: isospin antisymmetric, spin symmetric



reviews: Afanasjev, Fifty years of Nuclear BCS, p.138, arXiv:1205.2134 Frauendorf and Macchiavelli, Prog. Part. Nucl. Phys. **78**, 24 (2014)

neutron-proton pairing condensation?

possible in proton-rich region (around N=Z)-- relevant to rp process Wigner energy



additional binding for even-even system

$$\Delta B = -E_W = -W(A)|N - Z|$$

A Satula et al., Phys. Lett. B 407, 103 (1997) isovector or isoscalar pair condensation?



red: isoscalar condensate blue: isovector np and isoscalar np mixture green: like-particle pairing condensate

Woods-Saxon + np pairing int. from shell model Hamiltonian

Gezerlis, Bertsch, Luo, Phys. Rev. Lett. 106, 252502 (2011)

Neutron-proton pairing

neutron-proton pairing as residual correlation (isoscalar pairing)

beta-decay rate (relevant to r-process)
double-beta decay

npQRPA calculation for beta decay

Yoshida, Prog. Theor. Exp. Phys. 2013, 113D02 (2013)

Iow-energy Gamow-Teller strength

npQRPA calculation f: relative strength of isoscalar np pairing (b) ⁵⁶Ni T21 (b) ⁵⁶Ni T21 (c) ¹ (c)



Bai et al. Phys. Lett. B 719, 116 (2013)

30 MeV

 $\mathsf{B}_{\mathsf{low}}/\mathsf{B}_{\mathsf{high}}$

0

DFT for np pairing condensation

nuclear DFT (and beyond): microscopic and global description of finite nuclei Most DFT calculations include np pairing only as residual correlation (npQRPA) Most calculations for np pair condensation use schematic interactions

DFTs with np pairing condensation

Terasaki, Wyss, and Heenen (Skyrme, Phys. Lett. B **437**, 1(1998)) Afanasjev and Frauendorf (RHB, Phys. Rev. C **71**, 064318 (2005))

Goal

develop a neutron-proton DFT code based on HFBTHO (Skyrme) and give a unified description for np pairing correlation and condensation

theoretical formalism:

"Local density approximation for proton-neutron pairing correlations: Formalism" Perlinska, Rohozinski, Dobaczewski, Nazarewicz Phys. Rev. C **69**,014316 (2004) (isospin-invariant EDF)

particle-hole implementation:

"Isospin-invariant Skyrme energy-density-functional approach with axial symmetry" Sheikh, NH, Dobaczewski, Nakatsukasa, Nazarewicz, Sato, Phys. Rev. C **89**, 054317 (2014)

Isospin representation of ph density

Perlinska et al., Phys. Rev. C 69,014316 (2004)

density matrix
$$\hat{\rho}(\mathbf{r}st, \mathbf{r}'s't') = \langle \Psi | a_{\mathbf{r}'s't'}^+ a_{\mathbf{r}st} | \Psi \rangle$$

non-local density $\rho_k(\mathbf{r}, \mathbf{r}') = \sum_{stt'} \hat{\rho}(\mathbf{r}st, \mathbf{r}'st') \hat{\tau}_{t't}^k$ $\hat{\tau}_{t't}^0 = \delta_{t't}$
local density $\rho_k(\mathbf{r}) = \rho_k(\mathbf{r}, \mathbf{r}') |_{\mathbf{r}=\mathbf{r}'}$
isoscalar $\rho_0(\mathbf{r}) = \rho_n(\mathbf{r}) + \rho_p(\mathbf{r})$ $\rho_n(\mathbf{r}) = \langle \Psi | a_n^+(\mathbf{r}) a_n(\mathbf{r}) | \Psi \rangle$
(conventional)
isovector $\rho_3(\mathbf{r}) = \rho_n(\mathbf{r}) - \rho_p(\mathbf{r})$ $\rho_p(\mathbf{r}) = \langle \Psi | a_p^+(\mathbf{r}) a_p(\mathbf{r}) | \Psi \rangle$
new densities present only when neutron-proton symmetry is broken
 $\rho_1(\mathbf{r}) = \rho_{np}(\mathbf{r}) + \rho_{pn}(\mathbf{r})$ $\rho_{pn}(\mathbf{r}) = \langle \Psi | a_n^+(\mathbf{r}) a_p(\mathbf{r}) | \Psi \rangle$

$$ho_2(oldsymbol{r}) = -i\{
ho_{np}(oldsymbol{r}) -
ho_{pn}(oldsymbol{r})\}$$

$$\rho_{np}(\mathbf{r}) = \langle \Psi | a_p^+(\mathbf{r}) a_n(\mathbf{r}) | \Psi \rangle$$

(time reversal symmetry cancels ρ_2)

Isospin representation allows us to have n-p mixed density

Isospin-invariant EDF (Skyrme)

isoscalar functional

Perlinska et al., Phys. Rev. C 69,014316 (2004)

$$\chi_0(\boldsymbol{r}) = C_0^{
ho} \rho_0^2(\boldsymbol{r}) \qquad
ho_0(\boldsymbol{r}) =
ho_n(\boldsymbol{r}) +
ho_p(\boldsymbol{r})$$

isovector functional (conventional) isovector functional (isospin-rotation invariant)

Isospin-invariant Skyrme functional (density bilinear, Ct^p is density dependent)

$$\begin{split} \chi_{0}(\boldsymbol{r}) &= C_{0}^{\rho} \rho_{0}^{2} + C_{0}^{\Delta\rho} \rho_{0} \Delta\rho_{0} + C_{0}^{\tau} \rho_{0} \tau_{0} + C_{0}^{J0} J_{0}^{2} + C_{0}^{J1} J_{0}^{2} + C_{0}^{J2} \underline{J}_{0}^{2} + C_{0}^{\nabla J} \rho_{0} \nabla \cdot \boldsymbol{J}_{0} \\ &+ C_{0}^{s} \boldsymbol{s}_{0}^{2} + C_{0}^{\Delta s} \boldsymbol{s}_{0} \cdot \Delta \boldsymbol{s}_{0} + C_{0}^{T} \boldsymbol{s}_{0} \cdot \boldsymbol{T}_{0} + C_{0}^{j} \boldsymbol{j}_{0}^{2} + C_{0}^{\nabla j} \boldsymbol{s}_{0} \cdot (\nabla \times \boldsymbol{j}_{0}) + C_{0}^{\nabla s} (\nabla \cdot \boldsymbol{s}_{0})^{2} + C_{0}^{F} \boldsymbol{s}_{0} \cdot \boldsymbol{F}_{0}, \\ \chi_{1}(\boldsymbol{r}) &= C_{1}^{\rho} \vec{\rho}^{2} + C_{1}^{\Delta\rho} \vec{\rho} \circ \Delta \vec{\rho} + C_{1}^{\tau} \vec{\rho} \circ \vec{\tau} + C_{1}^{J0} \vec{J}^{2} + C_{1}^{J1} \vec{J}^{2} + C_{1}^{J2} \underline{\vec{J}}^{2} + C_{1}^{\nabla J} \vec{\rho} \circ \nabla \cdot \vec{J} \\ &+ C_{1}^{s} \vec{s}^{2} + C_{1}^{\Delta s} \vec{s} \cdot \circ \Delta \vec{s} + C_{1}^{T} \vec{s} \cdot \circ \vec{T} + C_{1}^{j} \vec{j}^{2} + C_{1}^{\nabla j} \vec{s} \cdot \circ (\nabla \times \vec{j}) + C_{1}^{\nabla s} (\nabla \cdot \vec{s})^{2} + C_{1}^{F} \vec{s} \cdot \circ \vec{F}, \end{split}$$

Isovector part is extended to include np-mixing
 No new coupling constants in ph channel
 Coulomb functional breaks isospin invariance (not shown here)

Implementation to axial DFT solver HFBTHO

Sheikh et al. Phys. Rev. C 89, 054317 (2014)

Isobaric analogue states (IASs)



ground state with N neutrons and Z protons has isospin $T=T_z=(N-Z)/2$

 $|^{78}Ni(g.s)\rangle = |T=11, Tz=11\rangle$

isobaric analogue states: states with $T \neq \pm Tz$

 $|T=11,T_z=10> = T_{-}|^{78}Ni(g.s.)>$ isospin lowering operator $T_{-}= \Sigma p_i^+n_i$ IASs of ⁷⁸Ni (N=50, Z=28, T=11) found in excited states in ⁷⁸Cu (Tz=10), ⁷⁸Zn(Tz=9), ⁷⁸Ga(Tz=8), ⁷⁸Ge(Tz=7), ...

Implementation to axial DFT solver HFBTHO

Isobaric analogue states (IASs)

IASs are generated by applying T- to |T Tz=T>

superposition of mean fields

Sheikh et al. Phys. Rev. C 89, 054317 (2014)

mean-field description of IAS:

|T Tz> is the isospin T state with different orientation of the third component (orientation in isospace)

isospin rotation \rightarrow neutron-proton mixing in the single-particle states

isocranking

isocranking term $-\vec{\lambda}\circ\hat{\vec{t}}=-\lambda_x\hat{t}_x-\lambda_z\hat{t}_z$

 $\hat{h}' = \hat{h} - \vec{\lambda} \circ \vec{t},$

tx, tz: isospin operators $\lambda x = 0$: normal HF calculation

 $\frac{\theta}{\theta'=180^{\circ}} \xrightarrow{\lambda z} \theta'=0^{\circ}$

λX

isorotation about y axis

$$\begin{pmatrix} \rho_0(\theta') \\ \rho_1(\theta') \\ \rho_2(\theta') \\ \rho_3(\theta') \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos \theta' & 0 & \sin \theta' \\ 0 & 0 & 1 & 0 \\ 0 & -\sin \theta' & 0 & \cos \theta' \end{pmatrix} \begin{pmatrix} \rho_0(0^\circ) \\ \rho_1(0^\circ) \\ \rho_2(0^\circ) \\ \rho_3(0^\circ) \end{pmatrix} \begin{array}{c} \rho_0(\mathbf{r}) = \rho_n(\mathbf{r}) + \rho_p(\mathbf{r}) \\ \rho_1(\mathbf{r}) = \rho_{np}(\mathbf{r}) + \rho_{pn}(\mathbf{r}) \\ \rho_3(\mathbf{r}) = \rho_n(\mathbf{r}) - \rho_p(\mathbf{r}) \end{array}$$

A=78 isobaric analog states Sheikh et al. Phys. Rev. C 89, 054317 (2014) A=78 T=11 states, from ⁷⁸Ni to ⁷⁸Sn without Coulomb EDF is isospin invariant; ⁷⁸Sn bound with Coulomb proton drip line (for T=11 IAS) at 78 Zr (T_z=-1) single-particle energies 10 $\langle \hat{ au}_z angle$ A=78, T≈11 $\langle \hat{\tau}_z \rangle$ A=78, T≈11 w/o Coulomb 1.0 1.0 0.8 energies (MeV) 0.8 -100.6 s.p. Routhians (MeV 0.6 -20 0.4 0.4 -200.2 0.2 -30 0.0 -30 0.0 -0.2 -0.2 -40 s.p. -0.4 -0.4 -50 -0.6 -0.6 -50-0.8 -0.8 w/ Coulomb -60^L -1.0-60L 30 120 150 180 60 90 -1.0 30 120 150 180 60 90 θ (deg) ⁷⁸Ni 78Sn θ (deg) 78Ni ⁷⁸Sn

mean-field description of IASs with neutron-proton mixing neutron-proton pairing in IASs?

pp densities in isospin representation

pair density matrix
$$\hat{\kappa}(\mathbf{r}st, \mathbf{r}'s't') = \langle \Psi | a_{\mathbf{r}'s't'}a_{\mathbf{r}st} | \Psi \rangle$$

 $\hat{\rho}(\mathbf{r}st, \mathbf{r}'s't') = -2s' \langle \Psi | a_{\mathbf{r}'-s't'}a_{\mathbf{r}st} | \Psi \rangle$ (time reversal)
 $\hat{\rho}(\mathbf{r}st, \mathbf{r}'s't') = 4s't' \langle \Psi | a_{\mathbf{r}'-s'-t'}a_{\mathbf{r}st} | \Psi \rangle$ (isospin symm.)
non-local pp density $\check{\rho}_k(\mathbf{r}, \mathbf{r}') = \sum_{stt'} \hat{\rho}(\mathbf{r}st, \mathbf{r}'st')\hat{\tau}_{t't}^k$
local pp density $\check{\rho}_k(\mathbf{r}) = \check{\rho}_k(\mathbf{r}, \mathbf{r}')|_{\mathbf{r}=\mathbf{r}'}$
 $\check{\rho}_n(\mathbf{r}) = \langle \Psi | a_n(\mathbf{r})a_n(\mathbf{r}) | \Psi \rangle$ $\check{\rho}_1(\mathbf{r}) = \check{\rho}_n(\mathbf{r}) + \check{\rho}_p(\mathbf{r})$
 $\check{\rho}_p(\mathbf{r}) = \langle \Psi | a_p(\mathbf{r})a_p(\mathbf{r}) | \Psi \rangle$ $\check{\rho}_2(\mathbf{r}) = i[\check{\rho}_n(\mathbf{r}) - \check{\rho}_p(\mathbf{r})]$

isovector np pairing

$$raket{
ho}_{np}(m{r}) = \langle \Psi | a_{
m n}(m{r}) a_{
m p}(m{r}) - a_{
m p}(m{r}) a_{
m n}(m{r}) | \Psi
angle \qquad raket{
ho}_{3}(m{r}) = 2raket{
ho}_{
m np}(m{r}) \ raket{
ho}_{0}(m{r}) = 0 \qquad ext{(Pauli principle)}$$

non-local spin pp density $\breve{s}_k(r, r') = \sum_{ss'tt'} \hat{\breve{\rho}}(rst, r's't') \sigma_{s's} \hat{\tau}_{t't}^k$ local pp spin density $\breve{s}_0(r) = \breve{s}_0(r, r') |_{r=r'}^{ss'tt'} = \breve{s}_{np}(r)$ k=1-3 zero due to Pauli principle (isoscalar pairing)

Isospin-invariant pairing EDF

isovector pairing functional (conventional)

$$\breve{\chi}_{\mathrm{n}}(\boldsymbol{r}) = \breve{C}_{\mathrm{n}}^{
ho}[
ho_{0}]|\breve{
ho}_{\mathrm{n}}(\boldsymbol{r})|^{2}$$

 $reve{\chi}_{\mathrm{p}}(oldsymbol{r}) = reve{C}_{\mathrm{p}}^{
ho}[
ho_{0}]|reve{
ho}_{\mathrm{p}}(oldsymbol{r})|^{2}$



Perlinska et al., Phys. Rev. C 69,014316 (2004)

isovector pairing functional (isospin-rotation invariant)

$$egin{aligned} ec{\chi}_1(m{r}) &= ec{C}_1^
ho[
ho_0]\{|ec{
ho}_1(m{r})|^2 + |ec{
ho}_2(m{r})|^2 + |ec{
ho}_3(m{r})|^2\}\ &= ec{C}_1^
ho[
ho_0]ec{
ho}^*(m{r}) \circ ec{
ho}(m{r}) \end{aligned}$$

k= 3 neutron-proton pairing terms

isoscalar pairing functional (np)

 $raket{\chi_0(m{r})=raket{C}_0^s[
ho_0]|raket{s}_0(m{r})|^2}$

A=48 isobaric analog states (w/o Coulomb)

A=48 T=4 states, from ⁴⁸Ca to ⁴⁸Ni w/o Coulomb: with artificially strong pairing (Δn , $\Delta p \neq 0$)

calculation starting from ⁴⁸Ca with proton gauge angle at ⁴⁸Ca $\phi = 0^{\circ}, 30^{\circ}, 60^{\circ}, \dots, 150^{\circ}, 180^{\circ}$ ($\Delta_{p} \sim |\Delta_{p}|e^{i\phi}$)

gauge angle

U(1) phase degree of freedom introduced with gauge symmetry breaking by pairing condensation



Isospin rotation about 2-axis

$$\begin{array}{l} \text{ph density} \begin{pmatrix} \rho_{0}(\theta') \\ \rho_{1}(\theta') \\ \rho_{2}(\theta') \\ \rho_{3}(\theta') \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos \theta' & 0 & \sin \theta' \\ 0 & 0 & 1 & 0 \\ 0 & -\sin \theta' & 0 & \cos \theta' \end{pmatrix} \begin{pmatrix} \rho_{0}(0^{\circ}) \\ \rho_{1}(0^{\circ}) \\ \rho_{2}(0^{\circ}) \\ \rho_{3}(0^{\circ}) \end{pmatrix} \begin{pmatrix} \rho_{0}(\mathbf{r}) = \rho_{n}(\mathbf{r}) + \rho_{p}(\mathbf{r}) \\ \rho_{3}(\mathbf{r}) = \rho_{n}(\mathbf{r}) - \rho_{p}(\mathbf{r}) \\ \rho_{3}(\mathbf{r}) = \rho_{n}(\mathbf{r}) - \rho_{p}(\mathbf{r}) \\ \hline \rho_{1}(\mathbf{r}) = \rho_{n}(\mathbf{r}) - \rho_{n}(\mathbf{r}) \\ \hline \rho_{1}(\mathbf{r}) = \rho_{n}(\mathbf{r}) \\ \hline \rho_{1}(\mathbf{r}) = \rho_{n}(\mathbf{r}) - \rho_{n}(\mathbf{r}) \\ \hline \rho_{1}(\mathbf{r}) = \rho$$

k=1 pair density depends on the relative gauge angle



infinitesimally degenerated solutions with isospin symmetry of EDF

A=48 isobaric analog states (w/ Coulomb)

A=48 T=4 states, from ⁴⁸Ca to ⁴⁸Ni w/ Coulomb: isospins symmetry of the EDF broken solutions with ϕ =0° and 180° survive during the isospin rotation

pairing energy(n,p,np)

pairing energy(1,2,3)



Almost degenerated two solutions in IASs with pairings (with Coulomb) Coulomb prefers like-particle pairing solution degree of freedom connecting these two would be important kink around θ '~100° is due to the pairing cutoff

energy at $\theta'=90^{\circ}$ $\phi=0^{\circ}$ -387.115215 MeV $\phi=180^{\circ}$ -387.103344 MeV Neutron-proton condensation in ground states

results: difficult to get convergence(!)

if the potential energy surface is close to constant, finding an energy minimum is very difficult

constraints on pairing amplitudes for PES calculations

$$\hat{S}_{k} = \int d\boldsymbol{r} \sum_{stt'} 4st' \hat{a}_{\boldsymbol{r}-\boldsymbol{s}-t'} \hat{a}_{\boldsymbol{r}st} \hat{\tau}_{t't}^{k} \qquad \langle \hat{S}_{k} \rangle = \int d\boldsymbol{r} \breve{\rho}_{k}(\boldsymbol{r})$$

<S₃>: neutron-proton pairing amplitude

 $<S_3>=0$: (with $<S_1>$ or $<S_2>\neq0$) like-particle condensation $<S_3>\neq0$: isovector np pair condensation

isovector np pair condensation in N=Z

parameter choice: spherical and large pairing (non realistic) A=68, T_z=0, without Coulomb, Q₂ = 0 (spherical), $<S_2>=0$ (SkM*, N_{sh}=7, C₁^ρ=-1224 MeV fm³)



 $g_{pp}=1$ (isospin-invariant EDF)

degenerated solutions along $|\langle S_1 \rangle|^2 + (|\langle S_2 \rangle|^2) + |\langle S_3 \rangle|^2 \sim 15.5^2$ $g_{pp} > 1$:

 $<S_1>=0$ and $<S_3>\neq 0$ HFB solution (np condensation)

PES from $\langle S_3 \rangle = 0$ to ~ 15.5 corresponds to isospin rotation

Effect of Coulomb





Coulomb does not prefer isovector np condensation

Realistic calculations

UNEDF1-HFB functional, N_{sh}=10 O to Sn isotopes around N=Z

Three sources of isospin symmetry breaking

- 1) particle-hole Coulomb functional
- 2) difference in nn and pp pairing strength
- 3) g_{pp} difference between isovector nn-pp and np pairing strength



■ Approximate isospin symmetry holds for isovector pairing with 1) and 2) ■ Isovector np-pair condensed solution found in 64 Ge (g_{pp}=1.0)

Realistic calculations (64Ge)

Pairing energy: isospin-symmetry breaking component very small



Isoscalar pairing

isoscalar pairing

- no evidence for isoscalar np pair condensation
- □ strength globally fitted to beta decay rate (QRPA)
 - Mustonen and Engel, Phys. Rev. C 93, 014304 (2016)
- double-beta decay (QRPA, no global fit completed)





both rates (nuclear matrix element) depend strongly on isoscalar pairing \rightarrow include available $2\nu\beta\beta$ data for global fit of isoscalar pairing strength

Double-beta decay in nuclear DFT



standard DFT approach: diagonalization (computationally demanding) finite-amplitude method (linear response theory, iteration)



NH, AIP Conf. Proc. 2165, 020010 (2019)

Test calculation for ⁴⁸Ca→⁴⁸Ti

isovector np pairing dependence on double-Fermi, 2vββ Fermi matrix element



isoscalar np pairing dependence on double-GT, 2vßß Gamow-Teller matrix element



NH, AIP Conf. Proc. 2165, 020010 (2019)

 $2\nu\beta\beta$ experimental value :

 $M_{2v} = 0.046 \pm 0.004 \text{ MeV}^{-1}$ (Barabash, Nucl. Phys. A 935, 52 (2015), with $g_A = 1.27$)

Summary

- Neutron-proton DFT based on HFBTHO has been implemented
 - degenerated solutions are found in isobaric analogue states with isovector pairing
 - ⁶⁴Ge ground state is found to be isovector np pairing condensation in UNEDF1-HFB functional
- Isospin symmetry is still approximately good with Coulomb and like-particle pairing (with Vn≠Vp)
- Beyond mean field treatment to include isospin rotation degrees of freedom is necessary to include correlation (isospin projection?)
- New technique to calculation 2vββ nuclear matrix element to be used to determine the strength of isoscalar pairing
- Collaborators: Javid Sheikh(Kashmir, India), Witek Nazarewicz (MSU), Jacek Dobaczewski (York, UK), Jon Engel (UNC-CH)