Symmetry restoration in the mean-field description of proton-neutron pairing

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September 3, 2019

Recent advances on proton-neutron pairing, ESNT 2-6 September 2019

Table of contents

Introduction

Motivation

- Proton-neutron (pn) pairing correlations have been largely neglected in most of the calculations in nuclear structure.

[1] Frauendorf, S., Macchiavelli, A. O. (2014). Overview of np pairing. PPNP, 78

[2] Rrapaj, Ermal, Macchiavelli A.O., and Gezerlis A. Symmetry restoration in mixed-spin paired heavy nuclei. PRC 99.1 (2019)

[3] Perliska, E., et al. "Local density approximation for pn pairing correlations:

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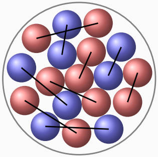
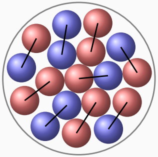
- Proton-neutron (pn) pairing correlations have been largely neglected in most of the calculations in nuclear structure.
- Coexistence between proton-neutron (isoscalar) and like-particle (isovector) condensates is expected to appear in $N = Z$ nuclei[1].



Isovector condensate



Isoscalar-isovector coexistence

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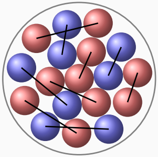

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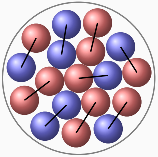

Isoscalar-isovector coexistence

- The aforementioned coexistence is elusive[2] and "no symmetry-unrestricted mean-field calculations of pn pairing with an isospin conserving formalism have been carried out"[3].

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$SO(8)$ solvable model

Pairing Hamiltonian:

$$\hat{H} = \overbrace{-g(1-x)\sum_{\nu} \hat{P}^{\dagger}_{\nu}\hat{P}_{\nu}}^{\text{Isovector contribution}} \underbrace{-g(1+x)\sum_{\mu} \hat{D}^{\dagger}_{\mu}\hat{D}_{\mu}}_{\text{Isoscalar contribution}}$$

Pang, Sing Chin. "Exact solution of the pairing problem in the LST scheme." Nuclear Physics A 128.2 (1969): 497-526.

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$$\hat{P}_{\nu}^{\dagger} = \sqrt{\frac{2l+1}{2}}\left(a_{l\frac{1}{2}\frac{1}{2}}^{\dagger}a_{l\frac{1}{2}\frac{1}{2}}^{\dagger}\right)_{M=0,S_z=0,T_z=\nu}^{L=0,S=0,T=1} \tag{1}$$

$$\hat{D}_{\mu}^{\dagger} = \sqrt{\frac{2l+1}{2}}\left(a_{l\frac{1}{2}\frac{1}{2}}^{\dagger}a_{l\frac{1}{2}\frac{1}{2}}^{\dagger}\right)_{M=0,S_z=\mu,T_z=0}^{L=0,S=1,T=0} \tag{2}$$

x: mixing parameter, g: strength of the interaction.

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Mean-field description and beyond

Hartree-Fock-Bogoliubov (HFB) formalism

Starting point: HFB calculation, by means of a transformation from the single-particle basis $(\hat{a}, \hat{a}^\dagger)$ to the quasiparticle basis $(\hat{\beta}, \hat{\beta}^\dagger)$

$$\hat{\beta}_i^\dagger = \sum_k u_{ik}\hat{a}_i^\dagger + v_{ik}\hat{a}_i \longrightarrow \hat{\beta}|\Psi\rangle = 0$$

including spin and isospin mixing. By means of the Thouless theorem, we include the contribution from each correlated pair in the wavefunction

$$|\Psi\rangle = \mathcal{N}\exp\left(\hat{Z}^+\right)|0\rangle \tag{3}$$

with

$$\hat{Z}^+ = \sum_{\nu=\pm1,0} p_\nu \hat{P}_\nu^+ + \sum_{\mu=\pm1,0} d_\mu \hat{D}_\mu^+ \tag{4}$$

Ring, Peter, and Peter Schuck. The nuclear many-body problem. Springer Science & Business Media, 2004.

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$$p_0 = \sin(\alpha/2)e^{-i\varphi}, \quad d_0 = \cos(\alpha/2)e^{i\varphi} \tag{5}$$

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The resulting HFB energy being $E = \langle\Psi|\hat{H}|\Psi\rangle$

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HFB results[4]

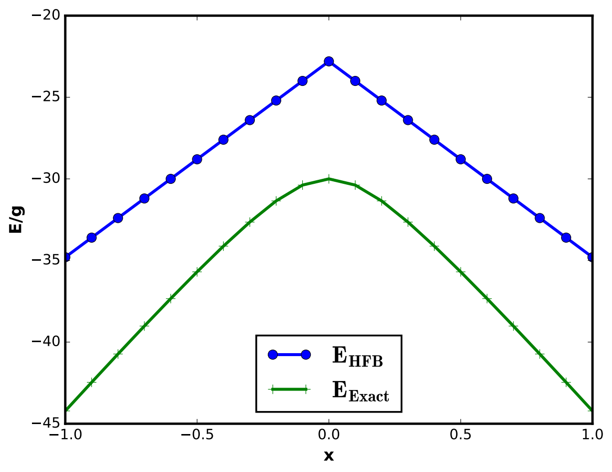

Figure 1: Energy (arbitrary units) as a function of the tuning parameter x for a model-space with $l = 2$, $A = 12$ obtained from the HFB and exact solutions.

[4] A.M. Romero, J. Dobaczewski, A. Pastore. APPB 49.3 2018

HFB results

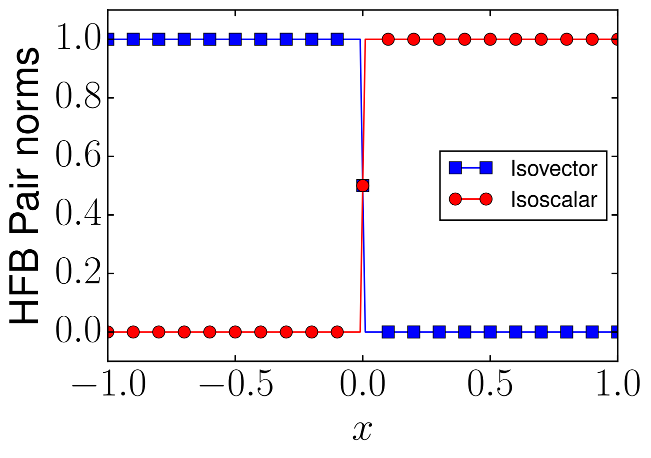

Figure 2: Normalised "number of pairs" as a function of the tuning parameter x computed using the HFB method.

Beyond mean-field: restoration of broken symmetries

The quasiparticle vacuum $|\Psi\rangle$ is a superposition of states with good particle (A), spin (S) and isospin (T) numbers, $|\Psi\rangle = \sum_{AST} c_{AST}|AST\rangle$, leading to broken symmetries.

Sheikh, J. A., et al. "Symmetry restoration in mean-field approaches." arXiv:1901.06992 (2019).

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$$|AST\rangle = \hat{P}^A \hat{P}^S \hat{P}^T |\Psi\rangle,$$

with

$$\hat{P}^A|\Psi\rangle = \frac{1}{2\pi}\int_0^{2\pi} d\varphi e^{i\varphi(\hat{A}-A)}|\Psi\rangle \tag{6}$$

$$\hat{P}^S_{S'_z S_z}|\Psi\rangle = \frac{2S+1}{8\pi^2}\int d\Omega_S D^{S*}_{S'_z S_z}(\Omega_S)\hat{R}(\Omega_S)|\Psi\rangle \tag{7}$$

$$\hat{P}^T_{T'_z T_z}|\Psi\rangle = \frac{2T+1}{8\pi^2}\int d\Omega_T D^{T*}_{T'_z T_z}(\Omega_T)\hat{R}(\Omega_T)|\Psi\rangle \tag{8}$$

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and the "projected energy" is calculated as

$$E_{\text{proj}} = \frac{\langle\Psi|\hat{H}|AST\rangle}{\langle\Psi|AST\rangle}$$

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Choice: variate, then project; or project, then variate?

We find two options to perform beyond mean-field calculations,

- Projection after variation (PAV):

$$\delta \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \bigg|_{|\Psi_{\mathsf{PAV}}\rangle} = 0 \longrightarrow E_{\mathsf{proj}}^{\mathsf{PAV}} = \frac{\langle \Psi_{\mathsf{PAV}} | \hat{H} | AST \rangle}{\langle \Psi_{\mathsf{PAV}} | AST \rangle}$$

- Variation after projection (VAP):

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As these methods rely upon the variational principle, the VAP approach should perform better.

Signature of the states

- States of good quantum numbers $|AST\rangle$ are also eigenstates of the signature operators in spin and isospin space

$$\hat{R}_S(\pi) = e^{-i\pi\hat{S}_y} \quad \hat{R}_T(\pi) = e^{-i\pi\hat{T}_y} \tag{9}$$

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$$\hat{R}_S(\pi)\hat{R}_T(\pi)|ST\rangle = (-1)^{S+T}|ST\rangle \tag{10}$$

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$$\hat{R}_S(\pi)\hat{R}_T(\pi)|A\rangle = \hat{R}_S(\pi)\hat{R}_T(\pi)\frac{(\hat{Z}^+)^{A/2}}{(A/2)!}|0\rangle = (-1)^{A/2}|A\rangle \tag{11}$$

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- Selection rule for the projected states:
  - If $S + T =$ even $\longrightarrow A/2 =$ even
  - If $S + T =$ odd $\longrightarrow A/2 =$ odd

Results

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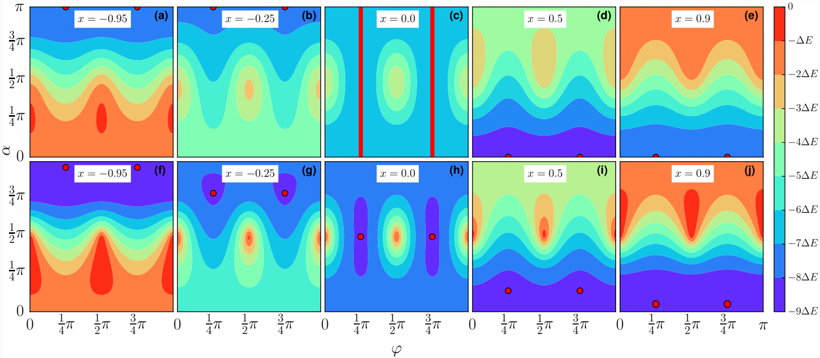


Figure 3: HFB (top) and VAP (bottom) energy (arbitrary units) surface as a function of the parameters α and φ for different values x of the interaction, for $S = T = 0$ and for a model-space with $\Omega = \sum_l (2l+1) = 12$, $A = 24$. Steps of $\Delta E = 20$, 15, 13, 17 and 20, respectively.

Energy

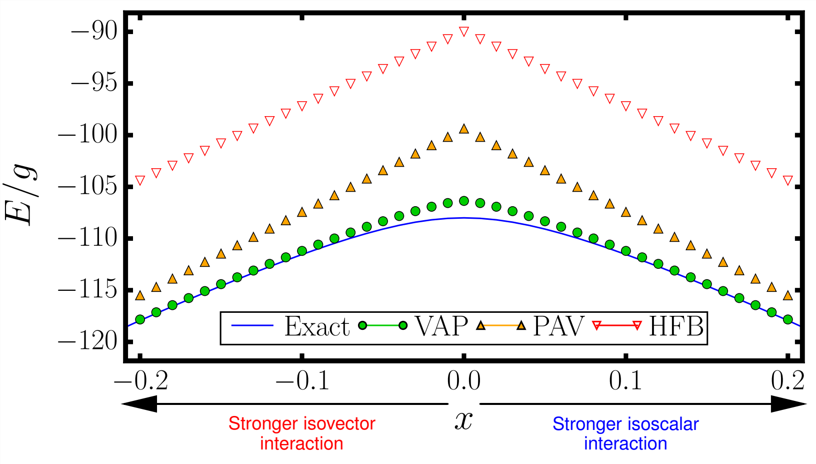
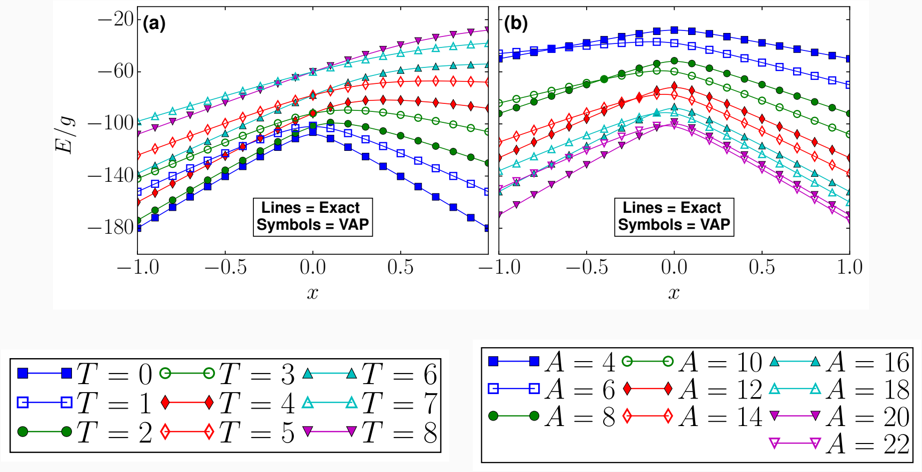
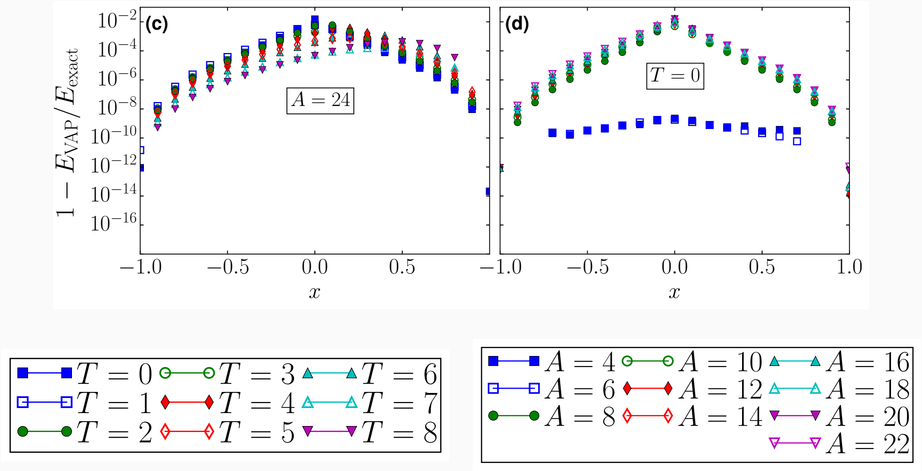


Figure 4: Energy (arbitrary units) as a function of the tuning parameter x for a model space with spatial degeneracy $\Omega = 12$ and $A = 24, S = T = 0$, obtained for HFB, PAV and VAP methods and comparing them to the exact solutions.

Energy: exact and VAP comparison



Differences



Pairing coexistence seen by the VAP approach!

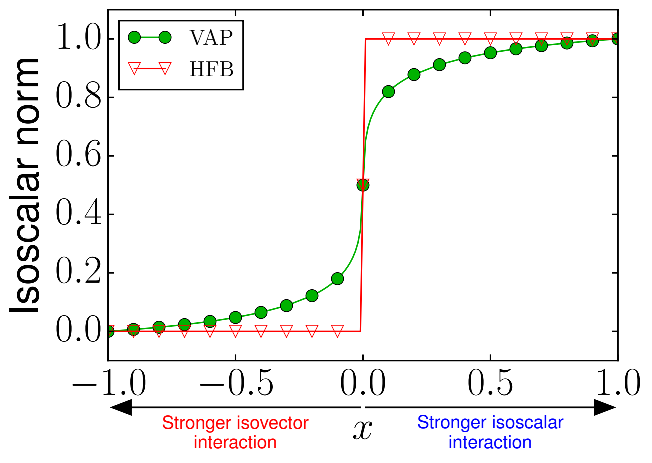
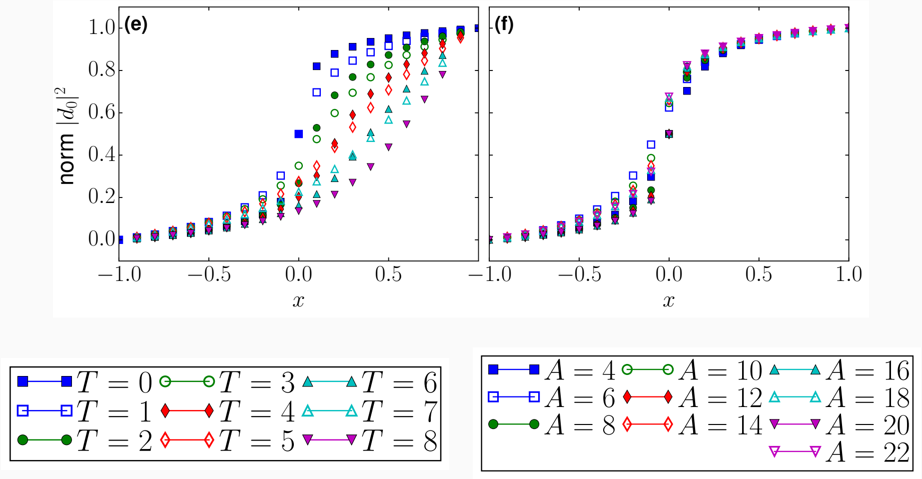
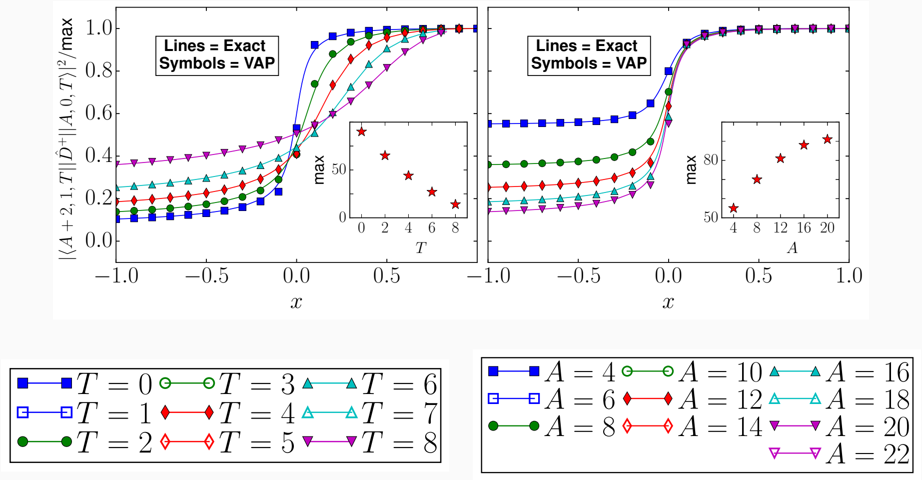


Figure 5: Norm of isoscalar pairs (contribution to the total wavefunction of the nucleus) as a function of the tuning parameter x obtained from VAP and PAV (HFB) methods.

Pairing coexistence for different A, S, T

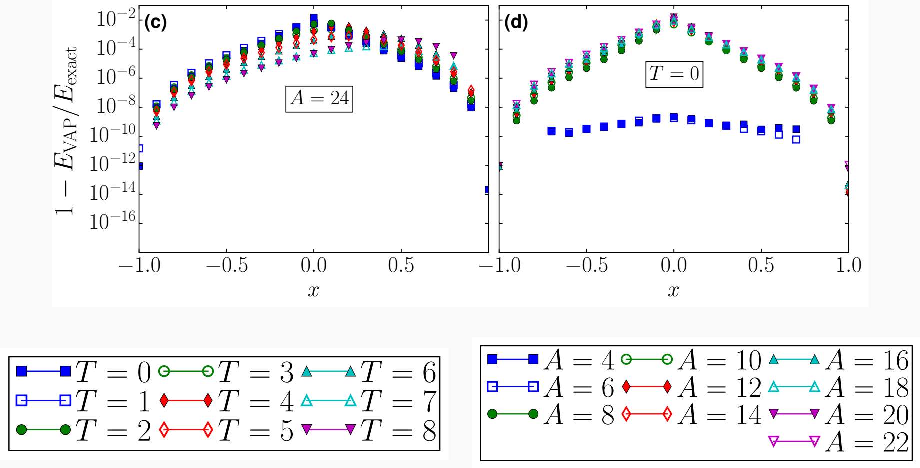


Deuteron transfer, the link between theory and experiment



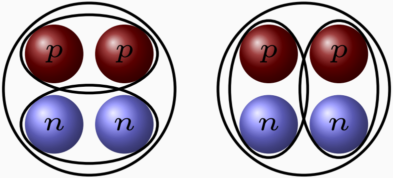
$A = 4$ and $A = 6$ cases

Differences



Projection gives exact states!

For $A = 4$, $S = T = 0$, there are only two possible configurations:



$\mathbf{(a)}$ $\mathbf{(b)}$

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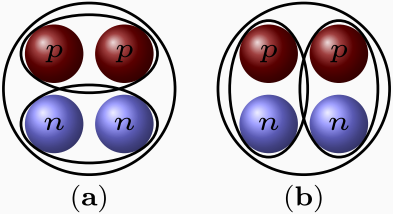

$$|A = 4, S = T = 0\rangle = \left[\alpha\left(\hat{P}^{+}\hat{P}^{+}\right)^{S=0,T=0} + \beta\left(\hat{D}^{+}\hat{D}^{+}\right)^{S=0,T=0}\right]|0\rangle \tag{13}$$

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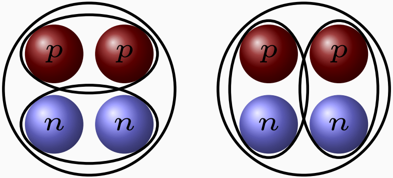

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For $A = 6$,

$$|A = 6, S = 1, T = 0\rangle = \hat{D}_0^{+}|A = 4, S = T = 0\rangle \tag{14}$$

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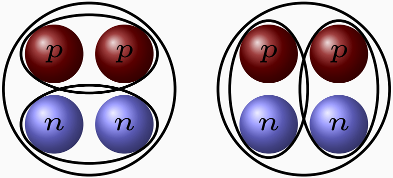

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For $A = 6$,

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No longer true for $A > 6$. It is not possible to describe those states entirely with our isoscalar and isovector pairs.

Importance of the separate symmetry restorations

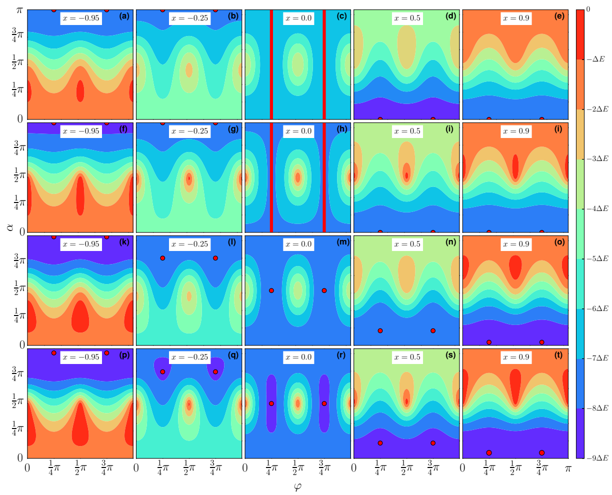

Figure 6: HFB (first row), particle-number restored (second row), spin plus isospin restored (third row) and particle number, spin and isospin restored (fourth row) energy surfaces.

Separable pairing

Realistic separable interaction in the pairing channel

$$V(\boldsymbol{r_1}, \boldsymbol{r_2}; \boldsymbol{r'_1}, \boldsymbol{r'_2}) = -\delta(X - X')\delta(Y - Y')\delta(Z - Z') \times P(x)P(y)P(z)P(x')P(y')P(z') \times [W + BP^\sigma - HP^\tau - MP^\sigma P^\tau] \tag{15}$$

where $\boldsymbol{r_i} = (x_i, y_i, z_i)$, $x = x_1 - x_2$ and $X = \frac{1}{2}(x_1 + x_2)$. The interaction is modelled by a Gaussian

$$P(x) = \frac{1}{\sqrt{4\pi}a} e^{-x^2/(4a^2)} \tag{16}$$

Realistic separable interaction in the pairing channel

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Benchmarked with the spherical code HOSPHE with D1 parametrization

a (fm)	W (MeV)	B (MeV)	H (MeV)	M (MeV)
0.636	-369	369	0	0

Realistic separable interaction in the pairing channel

$$
\begin{aligned}
V(\boldsymbol{r_1}, \boldsymbol{r_2}; \boldsymbol{r'_1}, \boldsymbol{r'_2}) = &-\delta(X - X')\delta(Y - Y')\delta(Z - Z') \\
&\times P(x)P(y)P(z)P(x')P(y')P(z') \\
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a (fm)	W (MeV)	B (MeV)	H (MeV)	M (MeV)
0.636	-369	369	0	0

Followed by implementation of isoscalar pairing and the symmetry-restoration methodology.

Conclusions

Summary and ongoing work

- Symmetry-restored mean-field techniques accurately describes the exact solution within a simple $SO(8)$ pairing interaction model and the coexistence of the isoscalar and isovector pair condensates.

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- Further studies are to be carried out using realistic interactions and shell structure settings.

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Thank you for your attention.

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