Variation approach for pair determination in nucleon pair approximation

Y. Lei (雷杨)∗1 and H. Jiang (姜慧)2

1School of National Defense Science and Technology, Southwest University of Science and Technology, Mianyang 621010, China
2School of Arts and Sciences, Shanghai Maritime University, Shanghai 201306, China

(Dated: August 22, 2019)

We proposed a pair-condensation variation approach to evaluate the importance of collective pairs, and determine their structure in low-lying states. Based on such a variation, the nucleon pair approximation (NPA) could avoid the collective-pair uncertainty, which the previous NPA calculations have suffered a lot. With the trial calculation for transitional $^{132}$Ba, we exemplify the ability of our variation approach. In detail, the variation provides similar quadrupole deformation parameters to the Hartree-Fock calculations, and highlights the role of the pairing correlation in the $\gamma$ softness of $^{132}$Ba, with non-axisymmetric deformation degree of freedom. It conclusively helps the NPA to decide which collective pair is essential for obtaining lower yrast level scheme and reproducing the $I = 10$ backbending. With the optimized condensation of neutron negative-parity pairs, we explain why the neutron negative-parity pairs have a large impact on the backbending behavior, and they are still not recommended. The collective-pair weights from the optimized pair condensation with cranking roughly have a positive correlation to the pair numbers in the NPA eigenstates with few exceptions, which reasonably establishes the validity of our variation approach.

PACS numbers:
Keywords:

I. INTRODUCTION

The nucleon pair approximation (NPA) [1] is an efficient truncation scheme of the Shell Model [2, 3]. Inspired by the shell-model-foundation study of the interacting boson model [4], the NPA usually adopts the positive-parity SD pairs with spins $r = 0\hbar$ and $2\hbar$, corresponding to the $sd$ bosons [5, 6]. With such few collective pairs (and of cause smaller model space), the resultant wave-functions usually provide a clearer vision to the key components of the nuclear low-lying structure in the shell-model framework. Especially, the NPA can be uniquely powerful for heavy or medium-heavy $O(6)$ nuclei in transitional region between spherical and well deformed shapes, because these nuclei are normally $\gamma$-soft with large shape uncertainty, and thus difficult to be interpreted with conventional mean-field theories, while non-truncated shell-model calculation for them still suffers the large model space.

Beside of SD pairs, the inclusion of additional pairs, e.g., $G$ pair with spin $4\hbar$ and positive parity, can significantly improve the NPA results, especially for some non-yrast state with larger spin or even negative parity $r$ [7, 8]. However, such a strategy is trivial at some degree, because more pairs mean larger model space, and more similar NPA description to shell-model one [11, 12]. One can always obtain a reasonable approximation of the Shell Model by arbitrarily including a huge set of collective pairs. This is against the key original intention of the NPA, which is to describe the nucleus with a simpler picture of limited but the most important collective pairs. Therefore, it’s crucial to apriori evaluate the importance of a certain collective pair before the actual NPA calculation.

Moreover, without a priori pair-importance evaluation, there could be some ambiguity about which collective pair(s) should be included in the NPA. For example, there is a $I = 10$ backbending in the $^{132}$Ba yrast band [14, 16]. Both $(\nu b_{11/2})^{-2}$ pair and negative-parity pairs, together with SD pairs, can reproduce this backbending, but with different NPA wavefunctions [17, 19]. There is still no conclusive consensus on which set of collective pairs is superior for this $I = 10$ backbending.

In the early 1980s, the Hartree-Fock-Bogolyubov (HFB) was frequently adopted to demonstrate the importance of the SDG pairs, and determine their structures in low-lying states (for example in Refs. [20, 21]). It’s possible that the HFB somehow could provide a pair-importance guide for the NPA. However, it still may not be the most applicable to realistic NPA calculations, from a modern point of view. First of all, the HFB violates the particle-number conservation, and only provides an average picture around the nucleus under investigation. In the transitional region, where the NPA is mostly adopted, the nuclear shape can develop dramatically from spherical to well deformed. Accordingly, the wavefunction, or the collective pairs in the NPA framework, should also evolve quickly as increasing valence particle number. An HFB variation averaging a few nearby nuclei may lead to an inaccurate description of the pair importance and structure. Secondly, previous pair-importance studies with the HFB mostly focus on axially deformation with a fixed $\gamma = 0$ or $60^\circ$. However, it’s desirable for the NPA to include, or at least have access to, complete $\gamma$ degree

*corresponding author: leiyang19850228@gmail.com
of freedom, which is crucial to understand the $\gamma$ softness, $\gamma$ instability, shape coexistence and mixing in the transitional nuclei. Thirdly, the HFB imposes the coupling of a single-particle state and its time-reversal state in the pair structure, which forbids negative-parity pairs. However, the negative-parity pairs could be also important in low-lying states of $A \sim 100, 132$ and 208 nuclei [18, 22]. This is because, in these nuclear regions, the intruder $g_{9/2}$, $h_{11/2}$ and $i_{13/2}$ neutron hole states have very low single-hole energy, and thus can be coupled with other single-particle orbits to construct low-energy negative-parity pairs. Therefore, it’s essential to develop a new method to determine the importance of collective pairs specified for the NPA.

This work suggests such a type of method based on a variational approach with collective-pair condensation. We do not impose a certain angular momentum on such a collective pair, which is different from conventional NPA formalism. We apply this method to the NPA calculation for $^{132}\text{Ba}$ as a test, because $^{132}\text{Ba}$ is a typical transitional nucleus with six valence protons and six valence neutron holes. Namely, it’s a touchstone for the NPA calculation. Moreover, the ambiguity of its $I = 10$ backbending is directly related to comparison between the importance of $(\nu h_{11/2})^{-2}$ pair and negative-parity pairs. Our variational approach may provide a new vision with respect to this issue.

II. PAIR CONDENSATION VARIATION

Our method starts with a collective pair condensation, which was originally introduced to construct microscopic wave-function with the O(6) symmetry, and then to simplify the Monte Carlo Shell Model calculation for $A \sim 132$ region [23, 24]. However, our formalism of overlap and Hamiltonian matrix element is different from those in Refs. [23, 24], as summarized in Appendix.

The “collective pair” mentioned above is defined as:

$$\Omega^\dagger = \frac{1}{2} \sum_{ij} \omega_{ij} C_i^\dagger C_j^\dagger,$$

$$\Omega = (\Omega^\dagger)^\dagger = \frac{1}{2} \sum_{ij} \omega_{ij} C_j C_i,$$  \hspace{1cm} (1)

where $C_i^\dagger$ and $C_j^\dagger$ are single-particle creation operators, the $i$ and $j$ represent all the quantum numbers to label single-particle states, and $\omega_{ij}$ is the structure coefficient of the $\Omega$ collective pair. We enforce $\omega_{ij} = -\omega_{ji}$ to insure the uniqueness of the $\omega_{ij}$ coefficient. Thus, all the $\omega_{ij}$ coefficients can be mapped into a skew-symmetric matrix $\omega$ as

$$\omega = \begin{pmatrix}
0 & \omega_{01} & \omega_{02} & \cdots \\
-\omega_{01} & 0 & \omega_{12} & \cdots \\
-\omega_{02} & -\omega_{12} & 0 & \cdots \\
\cdots & \cdots & \cdots & \cdots
\end{pmatrix}$$  \hspace{1cm} (2)

The anti-symmetry of the $\omega$ matrix is the key to speed up the matrix-element calculation of the collective-pair condensation with the BLAS (Basic Linear Algebra Subprograms) library [25]. Therefore, we always anti-symmetrize the coefficient matrix $\omega$ by $\tilde{\omega} = \frac{1}{2}(\omega - \omega^T)$, if it’s not skew-symmetric.

We also note that the collective pair defined above is not labeled with certain angular momentum, angular-momentum projection on principal axis, or even parity. Because there is no angular-momentum coupling, such defined collective pair is denoted by “uncoupled collective pair” in this paper, to distinguish it from conventional collective pair with angular momentum as a good quantum number in the NPA. One sees that the uncoupled collective pair includes all the two-body configuration degrees of freedom, which enables to equally evaluate the importance of all possible NPA collective pairs in a single variation.

The trial wave function of our variation is the condensation of the uncoupled collective pair as $(\Omega^\dagger)^N\rangle$, where $2N$ is the valence particle/hole number in the model space. Given Hamiltonian operator $H$, the Hamiltonian expectation value can be calculated with the formalism in Appendix. Our variation will minimize the Hamiltonian expectation value, and converge to the conditions of

$$\delta \left( \frac{\langle \Omega^N H (\Omega^\dagger)^N \rangle}{\langle \Omega^N (\Omega^\dagger)^N \rangle} \right) = 0$$  \hspace{1cm} (3)

There is many efficient algorithms for such multidimensional minimization. We adopt the Broyden-Fletcher-Goldfarb-Shanno algorithm [26, 29], which requires the first derivatives of the Hamiltonian expectation value.

In Eq. (A.12), we prove that the first derivatives of the matrix element $\langle \hat{O} \rangle$ along the direction of arbitrary $\Gamma$ pair reads

$$\frac{\partial \langle \Omega^N \hat{O} (\Omega^\dagger)^N \rangle}{\partial \delta_{\Gamma}} = N \langle \Gamma | \Omega^{N-1} (\hat{O} + \hat{O}^\dagger)(\Omega^\dagger)^N \rangle,$$  \hspace{1cm} (4)

where the $\hat{O}$ is an arbitrary linear operator. With Eq. (4), we can express first derivatives of Hamiltonian expectation value analytically as in Eqs. (A.13), (A.14) and (A.15).

Here, we note that from, our formalism presented in the Appendix does not introduce recursion, and thus a code based on it would have polynomial time complexity. The NPA formalism [30, 31], on the other hand, suffers recursion with exponential time complexity. Therefore, as increasing valence particle number, the computational time of the pair-condensation variation would increase more slowly than conventional NPA code, and thus it is a tolerable and actually more efficient burden for the NPA calculation.

Furthermore, with Eq. (4) and the conservation laws of Hamiltonian, one can readily prove that the variation
of \( \langle \Omega | ) \) condensation has three “self-consistent sym-
metries” as

1) seniority: if initial or intermediate \( \Omega \) has only \( S \) pair
component, the variation keeps \( \Omega \) away from other
non-S pair components.

2) angular-momentum projection: if initial or interme-
diate \( \Omega \) has fixed angular-momentum projection, this
projection will not be changed in the variation.

3) parity: if initial or intermediate \( \Omega \) is labeled with cer-
tain parity, the variation does not change the parity
or mix it with alternative parity any further.

One can perform a variation with spherical and axisym-
metric deformation, given the symmetries \([\text{I}]\) and \([\text{II}]\), re-
spectively. In our calculation, it’s also found that the op-
timized pair condensation does not maintain parity mix-
ture, which may be related to the symmetry \([\text{III}]\), but has
not yet been proved mathematically.

After the variation, we normalize the pair structure
coefficients, so that \( \sum r \delta | \omega | = 1 \). Then we follow
the procedure suggested by Ref. \([\text{32}]\) to determine the
quadrupole deformation parameters, and decompose the
uncoupled collective pair \( \Omega \) into a series of collective
pairs, which can be further adopted in the NPA cal-
culations.

To calculate the deformation parameters \( \beta \) and \( \gamma \), the
quadrupole operator are defined as \( Q^2 = e_x Q_x^2 + e_y Q_y^2 + e_z Q_z^2 \)
with commonly adopted effective charge \( e_x = 1 \) and
\( e_y = -1 \). Here, we take negative neutron effective
charge, because valence neutrons of \(^{132}\text{Ba}\) occupy hole
states in our calculation. The \( Q^2 \) matrix of the pair con-
densation \( \langle \Omega^1 | N \rangle \) in the Cartesian coordinate has three
eigenvalues with two degrees of freedom in the intrin-
sic frame. The \( \beta \) and \( \gamma \) parameters are related to these
eigenvalues by

\[
Q_1 = \sqrt{\frac{2\pi}{5}} \left[ \sqrt{3} (Q_2 + Q_{-2}) - \sqrt{2} Q_0 \right]
\]
\[
Q_2 = \sqrt{\frac{2\pi}{5}} \left[ -\sqrt{3} (Q_2 + Q_{-2}) - \sqrt{2} Q_0 \right]
\]
\[
Q_3 = 2 \sqrt{\frac{4\pi}{5}} Q_0
\]

with

\[
Q_0 = \frac{3}{2\pi} \sqrt{\frac{4\pi}{5}} \langle r^2 \rangle \beta \cos \gamma
\]
\[
Q_2 = \frac{3}{2\pi} \sqrt{\frac{4\pi}{5}} \langle r^2 \rangle \frac{\beta}{\sqrt{2}} \sin \gamma
\]

where \( Q_1, Q_2, Q_3 \) are the three eigenvalues of the \( Q^2 \) matrix.

The NPA calculations adopt collective pairs with a cer-
tain parity, angular momentum \( r \), and its projection to
principle axle \( M \), as defined by

\[
A_M^r = \sum_{a \leq b} \beta_{ab}^r A_M^r(a b), \quad A_M^r(ab) = \frac{(C_a^r x C_b^r)^r}{\sqrt{1 + \delta_{ab}}}, \quad (7)
\]

where the \( a \) and \( b \) present the single-particle quantum
numbers of spherical basis, \( \{ \langle ml \rangle \} \). If our uncoupled
collective pair \( \Omega \) is also defined beyond spherical single-
particle basis, then pairs structure coefficients \( \beta_{ab}^r \)
are determined with the orthogonality of Clebsch-Gordan
Coefficient as

\[
\beta_{ab}^r = \sqrt{1 + \delta_{ab}} \sum_{ij} \delta_{j_i, j} \delta_{j, j} \langle C_i M_{\nu} | C_j M_{\nu} \rangle \langle \rho_j | \omega_{ij} \rangle. \quad (8)
\]

We note that, due to the isotropy of our Hamiltonian,
the principle axe for the angular-momentum projection
is uncertain, and thus the \( \beta_{ab}^r \) coefficients are actually
varied as space rotation. This will lead to the linearly
dependence of the \( \{ \beta_{r}^M, \beta_{a}^M, \beta_{b}^M \} \) vectors with
different \( M \). (To simply our following description, such
vectors are denoted by \( \{ \beta^M \} \).) One can introduce a uni-
tary transformation to orthogonalize the \( \{ \beta^M \} \) vectors
into \( \{ \beta^K \} \) vectors so that \( \sum_{a < b} \beta_{ab}^K \beta_{ab}^K = 0 \) if \( K \neq K' \).

We adopt the \( \{ \beta^K \} \) vector as the pair-structure coeffi-
cients of collective pair with spin \( r \) in our following NPA
calculation.

Here, we note that, the \( K \) index is introduced to dis-
tinguish several linearly independent \( \{ \beta^K \} \) vectors. It’s
NOT a angular-momentum projection. Furthermore, it’s
readily proved that \( \sum_{r, K \neq K} \langle C_i M_{\nu} | C_j M_{\nu} \rangle^2 = \sum_{i, j} \langle \delta_{ij} \rangle^2 = 1 \),
which means the length square of \( \{ \beta^K \} \) vector corre-
sponds to the weight of corresponding collective pair \( A^r \)
in optimized uncoupled collective pair \( \Omega \). Namely, it can be
taken as a quantitative measure of the importance of the
collective pair \( A^r \).

III. TRAIL CALCULATIONS FOR \(^{132}\text{Ba}\)

In previous NPA calculations for \(^{132}\text{Ba}\) \([\text{17}, \text{19}]\),
the single-particle model space is limited within the 50-
82 shell. The single-particle motion of valence neu-
trons is described in hole states, so that our wavefunc-
tions involves fewer particles. Thus, our NPA calculation
also adopt such model space with six valence pro-
tons and six valence neutron holes in the 50-82 major
shell. Corresponding collective pair condensation reads
\( \langle \Omega^1 | (\Omega^1)^3 | \Omega^1 \rangle \), where \( \Omega^1 \) is a proton uncoupled
collective pair, and \( \Omega^1 \) is a neutron pair. We don’t consider
the proton-neutron collective pairs here, as neglected in
previous NPA calculations \([\text{17}, \text{19}]\), because the proton-
neutron correlation in the transitional \(^{132}\text{Ba}\) is not fully
developed.

Adopted phenomenological Hamiltonian reads

\[
H = - \sum_{\sigma = \pi, \nu} \sum_{j} \langle \varepsilon_{\sigma j} \rangle \hat{n}_{\sigma j} + \sum_{\sigma = 0, 2} G_{\sigma \sigma} \hat{P}_{\sigma}^{(s)} \cdot \hat{P}_{\sigma}^{(s)} + \kappa_{\sigma} \hat{Q}_{\sigma} \cdot \hat{Q}_{\sigma} + \kappa_{\pi \nu} \hat{Q}_{\pi} \cdot \hat{Q}_{\nu}, \quad (9)
\]
TABLE I: Hamiltonian parameters proposed by Ref. [17] in unit of MeV. The upper part of this table presents the single-particle (s.p.) energies; the lower part presents two-body interaction parameters. There are two different sets of two-body interaction parameters denoted by PAR-1 and PAR-2 for simplification.

| s.p.   | $s_{1/2}$ | $d_{3/2}$ | $d_{5/2}$ | $g_{7/2}$ | $h_{11/2}$ |
|--------|-----------|-----------|-----------|-----------|------------|
| $\varepsilon_\pi$ | 2.990 | 2.708 | 0.962 | 0.000 | 2.793 |
| $\varepsilon_\nu$ | 0.332 | 0.000 | 1.655 | 2.434 | 0.242 |

| two-body | $G_{0\pi}$ | $G_{2\pi}$ | $G_{0\nu}$ | $G_{2\nu}$ | $\kappa_\pi$ | $\kappa_\nu$ | $\kappa_{\pi\nu}$ |
|----------|------------|------------|------------|------------|-------------|-------------|----------------|
| PAR-1    | 0.130 | 0.030 | 0.130 | 0.026 | 0.045 | 0.065 | 0.070 |
| PAR-2    | 0.170 | 0.040 | 0.150 | 0.026 | 0.030 | 0.100 | 0.080 |

TABLE II: Minimum energies, deformation parameters and collective-pair weights of the optimized collective pair condensation with the Hamiltonian parameters listed in Table I. The minimum energy is presented in unit of MeV. Collective pairs with weight less than 0.1 are omitted here.

| $E_{min}$ | $\beta$ | $\gamma$ | $\gamma_0$ |
|-----------|--------|--------|-----------|
| $\text{neutron}$ | -12.334 | 0.106 | $< 10^{-4}$ |
| $\text{proton}$ | -12.334 | 0.106 | $< 10^{-4}$ |
| $I^\pi = 0^+ (S)$ | 0.463 | 0.463 |
| $I^\pi = 2^+ (D)$ | 0.453 | 0.453 |
| $I^\pi = 2^+ (D)$ | 0.489 | 0.489 |
| $\text{neutron}$ | -15.418 | 0.102 | 16° |
| $\text{proton}$ | -15.418 | 0.102 | 16° |
| $I^\pi = 0^+ (S)$ | 0.428 | 0.428 |
| $I^\pi = 2^+ (D)$ | 0.449 | 0.449 |

With the parameters listed in Table I we perform variations for the uncoupled collective pair condensation. The variation results are listed in Table II. Both PAR-1 and PAR-2 parameters favor close $\beta$ values $\sim 0.1$, but different $\gamma$s. Namely, the PAR-1 provides a prolate deformation, while the PAR-2 drives the nucleus into a triaxial deformation.

To understand the $\gamma$ softness of $^{132}$Ba, we further perform a shape-constrained variation across minima and along the $\gamma$ direction. The obtained potential energy surfaces are compared with those from the Hartree-Fock (HF) calculations in Fig. 1. Here, we adopt the Sherpa code [33] for our HF calculations. The global HF minimum local at ($\beta = 0.113$, $\gamma = 0^\circ$) and ($\beta = 0.116$, $\gamma = 12.9^\circ$) for PAR-1 and PAR-2, respectively. Such quadrupole deformations are similar to those from the pair-condensation variation as listed in Table II which supports the validity of our variation approach. On the other hand, the pair-condensation variation provides much more flat minima along the $\gamma$ direction than the HF does, and thus establishes the $\gamma$ softness of $^{132}$Ba. Therefore, the pairing correlation introduced in the pair condensation can be indispensable for the low-lying states of $\gamma$-soft nuclei.

From Table II we also note that the pair decomposition from both PAR-1 and PAR-2 are very similar. Most (over 85% weight) composition of the optimized $\Omega$ pairs is constructed with $SD$ pairs. This reemphasizes the importance of $SD$ pairs in low-lying states, as previous NPA calculations [11] already and frequently established. We introduce such $SD$ pairs into the NPA calculation and present the yrast level scheme in Fig. 2 compared with experiments and the NPA results beyond conventional determined $SD$ pairs from a numerical fitting to projected BCS wave-function (PBCS) [34]. Obviously, the pair-condensation variation leads to lower $0^+$, $2^+$, $4^+$ and even $6^+$ states than BPCS does. A reasonable
yrast states, we adopt a cranking Hamiltonian as
adjusting the rotational frequency
and introduce it into the minimization of Eq. (3). By
local minima with
\( \langle \) reaches 8\( ^+ \) and \( 10^+ \) states from experiment and the NPA calculations
with PCBS pairs local at the same level as highlighted with the dash horizontal line.

low-lying truncation scheme of the Shell Model should
provide as lower yrast levels as possible because lower energy empirically hints larger overlap between eigenstate
from truncated subspace and that from full shell-model space. Therefore, we believe that the pair structure from
our variation approach enhances the similarity between
low-lying NPA wave-functions and shell-model ones.

With only \( SD \) pairs as presented Fig. 2 the calculated \( 8^+ \) and \( 10^+ \) states are obviously higher than experiment. Empirically speaking, the reasonable description of \( I \geq 8 \) yrast states requires additional collective pairs, which agrees with previous calculations [17, 19]. To specify which additional collective pairs should work for \( I \geq 8 \) yrast states, we adopt a cranking Hamiltonian as

\[
H_{\text{crank}} = H - \omega_x J_x,
\]

and introduce it into the minimization of Eq. (5). By
adjusting the rotational frequency \( \omega_x \), we can obtain the local minima with
\( \langle J_x \rangle = \sqrt{I(I+1)} \) as proposed by Inglis [36]. With such a cranking variation, we present the pair-weight evolution as increasing the nuclear spin \( I \) in Fig. 3. Both PAR-1 and PAR-2 parameters are considered here, and lead to similar pair-weight evolution, as described follows. For spin \( I \leq 4 \), the \( SD \) pairs dominate the optimized pair condensation, while for \( I > 4 \) states, such dominance gradually vanishes. This explains why the \( SD \) NPA calculations have a better description for \( I \leq 4 \) states than that for larger \( I \) states, as established with Fig. 2. Especially, when \( I \) reaches \( 8\hbar \), the neutron \( H \) pair with spin \( r = 10 \) and \( \langle \nu h_{11/2} \rangle^{-2} \) configuration
takes over the dominance of neutron pair condensation.

On the other hand, for proton pair condensation, the contribution of the \( G \) and \( I \) collective pairs with \( r^\pi = 4^+ \)
and \( 6^+ \) becomes indispensable. We introduce the neutron \( H \) pair and proton \( G, I \) pairs into our NPA calculations, and compare the yrast level schemes with experiments and previously proposed NPA calculations [17, 18] as presented in Fig. 4. The structure coefficients of proton \( G \) and \( I \) pairs are from the cranking variation for \( I = 16 \) and 18, respectively, because the \( G \) and \( I \) pairs have a major contribution to the optimized pair condensation therein, as shown in Fig. 3.

In Fig. 4 with PAR-1 parameters, our pair-condensation variation provides far lower yrast level scheme than that with conventional collective pairs, especially for \( I \geq 6 \) states. Compared with PAR-1, the PAR-2 scenario is less dramatic, maybe because the previous NPA calculation with PAR-2 parameters already introduced the \( H \) pair [17]. However, our variation still remarkably leads to lower levels for all yrast states with PAR-2 parameters. More importantly, the \( I = 10 \) backbending is reproduced (the sudden drop of level space \( E_I - E_{I-2} \)) in all the four sets of NPA calculations, which demonstrates the introduction of cranking in our variation indeed is a feasible way to help the NPA with higher spin states.

In Ref. [18], we found that the inclusion of neutron negative-parity pairs may be an alternative way to describe the \( I = 10 \) backbending. However, the pair-condensation variation clearly suggests otherwise. To explain this conflict, we impose negative parity on the initial \( \Omega_p \) pair and then perform another set of cranking variations. According to the parity self-consistent symmetry described in Sec. [11] such variations definitely converges to a set of negative-parity neutron pairs. We plot energies and deformation parameters \( (\beta, \gamma) \) against spin \( I \) for such optimized condensation with negative-

![FIG. 2: \(^{132}\)Ba yrast level scheme from experiments [35] (labeled with “Exp.”) and \( SD \)-pair NPA calculations with PAR-1 and PAR-2 parameters. The “PCBS” label means that the adopted \( SD \) pairs are from an approximation of projected BCS as described in Ref. [53], and adopted in Refs. [18, 19]. “PVC” corresponds to the pair-condensation variation proposed in this paper. The energy scales are unified and shifted, so that 0\( ^+ \), 2\( ^+ \), 4\( ^+ \), 6\( ^+ \), and 8\( ^+ \) states are from an approximation of projected BCS as described in Ref. [34], and adopted in Refs. [18, 19].](image)

![FIG. 3: The pair-weight evolution as increasing spin \( I \), from the cranking pair-condensation variation. The upper panels is obtained with PAR-1 parameters, while the lower ones is with PAR-2. The left panels is for neutron pair weight, and the right is for proton.](image)
parity neutron pair, and compare them with those of global minima discussed above, as shown in Fig. 4. The minimal energies with negative-parity neutron pairs are systematically higher than that of global minima. This is why our variation does not suggest negative-parity pairs. However, we also note that, as the nuclear spin approaching the backbending around \( I = 10 \), the nuclear rotation drives two types of pair condensations to have closer minimal energies. On the other hand, such two optimized condensations have similar \( \beta \) parameters for all \( I \) values, while the \( \gamma \) parameters have larger divergence for low-spin \( I \). However, similarly to the minimal energies, the \( \gamma \) parameters of two optimized condensations will also get closer to each other around the backbending point. In a word, the negative-parity neutron pairs lead to more similar energy and deformation to the collective pairs emerging from cranking minima after crossing the backbending. This is why the negative-parity neutron pairs seem also capable of describing the yrast backbending. However, we remind that the neutron \( H \) and proton \( G \), \( I \) pairs are still superior to negative-parity pairs, as suggested by our variation.

To further demonstrate the validity of the pair-condensation variation, we calculate the pair numbers of \( G \), \( I \) and \( H \) pairs in the NPA eigenstates, and plot them against corresponding pair weight from pair-condensation variation with cranking, as shown in Fig. 6. By excluding three exceptional plots with \( I = 6 \), 8 for the \( G \) pair, and \( I = 12 \) for the \( H \) pair, rough systematics with positive correlation is established for both PAR-1 and PAR-2 parameters, as shown in Fig. 6. Namely, if some collective pair has a larger pair weight in the optimized (cranking) pair-condensation variation, it has more possibility to be important in (corresponding) NPA low-lying wavefunctions. Thus, we believe that the pair weight from the pair-condensation variation approach can be a priors and quantitative guide for the collective-pair selection before actual NPA calculation.

### IV. SUMMARY

The present work suggests a pair-condensation variation approach to improve the NPA calculations. Such variation has particle-number conservation, and thus can more accurately describe transitional nuclei, which the NPA are mostly applied to. It also includes all the two-body-configuration degrees of freedom. Therefore, it works for asymmetric deformed nuclei and is enable
to estimate the importance of negative-parity collective pairs. We also propose that such a variation has three self-consistent symmetries.

We perform a trial calculation for $^{132}\text{Ba}$, which is a typical transitional nucleus. The proposed variation approach is expected to well describe the nuclear shape, and, more importantly, improve the NPA calculation for $^{132}\text{Ba}$, as we have demonstrated. In detail, the variation provides a similar nuclear shape to the HF calculation, and more efficiently establishes the self-consistent symmetries.

Appendix: formalism for pair condensation

As in Refs. [23, 24], the contraction of two uncoupled collective pairs reads

$$[\Gamma, \Omega^\dagger] = -\frac{1}{2} tr(q) + Q \quad (A.1)$$

where $q$ is a matrix with $q = \omega^\gamma$, $tr(q)$ means the trace of $q$ matrix, and $Q$ is an one-body operator with the elements of matrix $q$ as its coefficients, i.e., $Q = q_{ij}a_i^\dagger a_j$.

The contraction of collective pair and an arbitrary one-body operator reads

$$[\Gamma, Q] = \frac{1}{2} \sum_{ijkl} \gamma_{ij}q_{kl} [a_ja_i, a_k^\dagger a_l] = \sum_{ijkl} q_{il} \gamma_{ij}a_ia_l,$$

If one lets $\Omega = [\Gamma, Q]$, then the coefficient matrix of $\Omega$ is $\omega = \gamma q + q^T \gamma$, where $q^T$ means the transposition of matrix $q$. Above two contraction would be frequently adopted in following formalism.

As in Refs. [23, 24], the overlap of the pair condensation $\langle \Omega^\dagger \rangle^N$ is denoted by $I^N$, and reads

$$I^N = \langle \Omega^N (\Omega^\dagger)^m \rangle = -\frac{1}{2} N \sum_{l=0}^{N-1} tr(\omega^{2l+2})J_l^{N-1}, \quad (A.2)$$

where

$$J_l^N = \left[ \frac{N!}{(N-l)!} \right]^2 I^{N-l} \quad (A.3)$$

To further calculate the Hamiltonian matrix element, we need the formalism of three other overlap as $\langle \Gamma^1 \Omega^{N-1} (\Omega^\dagger)^N \rangle$, $\langle \Gamma^1 \Gamma^2 \Omega^{N-2} (\Omega^\dagger)^N \rangle$, and $\langle \Gamma^1 \Gamma^2 \Gamma^3 \Omega^{N-3} (\Omega^\dagger)^N \rangle$, where $\Gamma^1$, $\Gamma^2$ and $\Gamma^3$ are arbitrary pairs with different coefficients matrix $\gamma^1$, $\gamma^2$ and $\gamma^3$ from each other and $\omega$ matrix. To simplify our formalism, these three overlap are denoted by $\langle \gamma^1, N \rangle$, $\langle \gamma^1, \gamma^2, N \rangle$, and $\langle \gamma^1, \gamma^2, \gamma^3, N \rangle$, respectively.

Refs. [23, 24] already provided

$$\langle \gamma^1, N \rangle = -\frac{1}{2} N \sum_{l=0}^{N-1} tr(\gamma^1 \omega^{2l+1}) J_l^{N-1} \quad (A.4)$$
Now let’s turn to a more complicated overlap $\langle \gamma^1, \gamma^2, N \rangle$

$$
\langle \gamma^1, \gamma^2, N \rangle = \sum_{l=0}^{N-1} \langle \Gamma^l \Omega^{N-2} (\Omega^l)^l [\Gamma^2, \Omega^l] (\Omega^l)^{N-1-l} \rangle + \frac{1}{2} N \text{tr}(\gamma^2 \omega) \langle \gamma^1, N-1 \rangle \\
+ N(N-1) \langle \Gamma^l (\Omega)^{N-2} (\Omega^l)^{N-2} \Gamma^{020} \rangle,
$$

where the $\Gamma^{020}$ pair has a coefficient matrix $\gamma^{020} = \omega \gamma^2 \omega$.

$$
\langle \Gamma^l \Omega^{N-2} (\Omega^l)^{N-2} \Gamma^{020} \rangle = \langle \Omega^{N-2} (\Omega^l)^{N-2} [\Gamma^1, \Gamma^{020}] \rangle + \sum_{l=0}^{N-3} \langle \Omega^{N-2} (\Omega^l)^l [\Gamma^1, \Omega^l] (\Omega^l)^{N-3-l} \Gamma^{020} \rangle
$$

$$
= -\frac{1}{2} \text{tr}(\gamma^1 \omega \gamma^2 \omega) J^{N-2} - \frac{1}{2} (N-2) \text{tr}(\gamma^1 \omega) \langle \omega \gamma^2 \omega, N-2 \rangle + (N-2)(N-3) \langle \omega \gamma^1 \omega, \omega \gamma^2 \omega, N-2 \rangle \\
+ (N-2) \langle \omega \gamma^1 \omega \gamma^2 \omega + \omega \gamma^2 \omega \gamma^1 \omega, N-2 \rangle.
$$

Combining above three equations, we have

$$
\langle \gamma^1 \gamma^2, N \rangle = -\frac{1}{2N(N-1)} \text{tr}(\gamma^1 \omega \gamma^2 \omega) J_2^N + \frac{1}{4} N(N-1) \text{tr}(\gamma^2 \omega) \sum_{l=0}^{N-2} \text{tr}(\gamma^1 \omega^{2l+1}) J_l^{N-2} \\
+ \frac{1}{4} N(N-1)(N-2)^2 \text{tr}(\gamma^1 \omega) \times \sum_{l=0}^{N-3} \text{tr}(\gamma^2 \omega^{2l+3}) J_l^{N-3} - N(N-1)(N-2)^2 \sum_{l=0}^{N-3} \text{tr}(\gamma^1 \omega \gamma^2 \omega^{2l+3}) J_l^{N-3} \\
+ N(N-1)(N-2)(N-3) \langle \omega \gamma^1 \omega, \omega \gamma^2 \omega, N-2 \rangle
$$

By solving above recursion relation, we can express the $\langle \gamma^1, \gamma^2, N \rangle$ overlap in terms of matrix traces and overlap-related $J$ tensor defined in Eq. (A.3) as

$$
-\frac{1}{2} N(N-1) \sum_{k=0}^{N-2-N/2} \left[ \frac{(N-2)!!(N-3)!!}{(N-2k)!!(N-2k-1)!!} \right]^2 \text{tr}(\gamma_1 \omega^{2k+1} \gamma_2 \omega^{2k+1}) J_2^{N-2k} \\
+ \frac{1}{4} N(N-1) \sum_{k=0}^{N-2-N/2} \left[ \frac{(N-2)!!(N-3)!!}{(N-2k-2)!!(N-2k-3)!!} \right]^2 \text{tr}(\gamma_2 \omega^{2k+1}) J_2^{N-2k-2} \\
+ \frac{1}{4} N(N-1) \sum_{k=0}^{N-3-N/2} \left[ \frac{(N-2)!!(N-3)!!}{(N-2k-3)!!(N-2k-4)!!} \right]^2 \text{tr}(\gamma_1 \omega^{2k+1}) J_2^{N-2k-3} \\
- N(N-1) \sum_{k=0}^{N-3-N/2} \left[ \frac{(N-2)!!(N-3)!!}{(N-2k-3)!!(N-2k-4)!!} \right]^2 \sum_{l=0}^{N-2k-3} \text{tr}(\gamma_1 \omega^{2k+1} \gamma_2 \omega^{2k+2l+3}) J_l^{N-2k-3}.
$$

where the % symbol is a remainder operator as in the C-language standard.
Following the same philosophy, we express $\langle \gamma^1, \gamma^2, \gamma^3, N \rangle$ as

$$\frac{1}{N(N-1)(N-2)} \sum_{t=0}^{N-3-N\%3} \left[ \frac{N!!(N-1)!!(N-2)!!}{(N-3t)!!(N-3t-1)!!(N-3t-2)!!} \right]^2 
\times \left[ \frac{1}{4} tr(\gamma_2\omega^{2t+1}) tr(\gamma_1\omega^{2t+1}t_{13}\omega^{2t+1}) - tr(\gamma_1\omega^{2t+1}t_{13}\omega^{2t+1}t_{13}\omega^{2t+1}t_{13}\omega^{2t+1}) \right] J_3^{N-3t} 
+ N(N-1)(N-2) \sum_{t=0}^{N-3-N\%3} \frac{1}{N-3t-3} \left[ \frac{(N-3)!!(N-4)!!(N-5)!!}{(N-3t-3)!!(N-3t-4)!!(N-3t-5)!!} \right]^2 
\langle \tilde{\gamma}, N - 3 - 3t \rangle$$

(A.9)

with

$$\tilde{\gamma} = \left[ \frac{1}{4} tr(\gamma_2\omega^{2t+1}) tr(\gamma_2\omega^{2t+1}) \right] \omega^{t+1} \gamma^{t+1} 
- \frac{1}{2} tr(\gamma_2\omega^{2t+1}) \omega^{t+1} \left[ \gamma_1\omega^{2t+1}t_{13} + t_{13}\omega^{2t+1} \gamma_1 \right] \omega^{t+1} + \omega^{t+1} \left[ t_{13}\omega^{2t+1}t_{13}\omega^{2t+1} \gamma_3 + t_{13}\omega^{2t+1} \gamma_3 \right] \omega^{t+1} 
- \frac{1}{2} tr(\gamma_2\omega^{2t+1}t_{13}\omega^{2t+1}) \omega^{t+1} \left[ \gamma_2\omega^{2t+1}t_{13} + t_{13}\omega^{2t+1} \gamma_2 \right] \omega^{t+1} 
+ \omega^{t+1} \left[ t_{13}\omega^{2t+1}t_{13}\omega^{2t+1} \gamma_3 + t_{13}\omega^{2t+1} \gamma_3 \right] \omega^{t+1}$$

For matrix element of an arbitrary one-body operator $Q$:

$$\langle Q^N Q (\Omega^l)^N \rangle = \sum_{l=0}^{N-1} \langle Q^l [\Omega, Q^l] Q^{N-l-1} (\Omega^l)^N \rangle = N \langle \omega q + q^T \omega, N \rangle = -N^2 \sum_{l=0}^{N-1} tr(q\omega^{2l+2}) J_3^{N-1}$$

(A.10)

One sees that, for any one-body operator $\langle Q^N Q (\Omega^l)^N \rangle = \langle Q^N Q^l (\Omega^l)^N \rangle$, considering the coefficient matrix of $Q^l$ is $q^T$, and $tr(q^T\omega^{2l+2}) = tr(q\omega^{2l+2})$. Therefore, if $Q$ is a spherical tensor, i.e., $(Q^l)^\dagger = (-)^l Q^{l\dagger}$, then odd $\kappa$ always leads to zero matrix element.

For matrix element of an arbitrary two-body operator $\Gamma^\dagger \Gamma$, where the $\Gamma$ pair has a coefficient matrix $\gamma$,

$$\langle \Omega^N \Gamma^\dagger \Gamma (\Omega^l)^N \rangle = \sum_{l=0}^{N-1} \langle \Omega^l [\Omega, \Gamma^\dagger] \Omega^{N-l-1} \Gamma (\Omega^l)^N \rangle = \frac{1}{2} N tr(\gamma) \langle \gamma, N \rangle + N(N-1) \langle \gamma, \omega \gamma, N \rangle,$$

(A.11)

For an arbitrary operator $\hat{O}$, the derivative of its matrix element along the direction of arbitrary $\Gamma$ pair reads

$$\frac{\partial \langle \Omega^N \hat{O}(\Omega^l)^N \rangle}{\partial \delta_{||\Gamma||}} = \lim_{\delta_{||\Gamma||} \to 0} \frac{\langle (\Omega + \delta_{||\Gamma||} \Gamma)^N \hat{O}(\Omega^l + \delta_{||\Gamma||} \Gamma)^N \rangle - \langle \Omega^N \hat{O}(\Omega^l)^N \rangle}{\delta_{||\Gamma||}}$$

$$= \lim_{\delta_{||\Gamma||} \to 0} \frac{\delta_{||\Gamma||} N \langle \Gamma (\Omega^{N-1} \hat{O} (\Omega^l)^N) + \delta_{||\Gamma||} N \langle \Omega^N \hat{O} (\Omega^l)^N \Gamma \rangle + O(\delta_{||\Gamma||}^2) \rangle}{\delta_{||\Gamma||}}$$

(A.12)

where $O(\delta_{||\Gamma||}^2)$ is the second infinitely small quantity of $\delta_{||\Gamma||}$.

In our variation, we choose all the $\omega_{ij}$s as our variables. With respect to a single matrix element $\omega_{kl}$, corresponding direction pair $\Gamma = \Omega^{kl}$ with coefficient matrix $\omega^{kl}$, and its matrix element $\omega_{kl} = \delta_{kl} \delta_{ij} - \delta_{jk} \delta_{il}$.
Let the \( \hat{O} \) to be an identity operator, Eq. (14) reduces to the first derivative of overlap \( I^N \) as

\[
\frac{\partial \langle \Omega^N (\Omega) \rangle}{\partial \omega_{kl}} = 2N \langle \omega^{kl}, N \rangle = 2N^2 \sum_{l=0}^{N-1} (\omega^{2l+1})_{kl} I^{N-1}. \tag{A.13}
\]

If \( \hat{O} = Q \), a one-body operator, then

\[
\frac{\partial \langle \Omega^N Q (\Omega) \rangle}{\partial \omega_{kl}} = N \langle \Omega^{kl} (\Omega)^{-1} (Q + Q^t)(\Omega) \rangle = N \langle [\Omega^{kl} Q + Q^t] \Omega^{-1} (\Omega) \rangle
\]

\[
+ N \sum_{l=0}^{N-2} \langle \Omega^{kl} Q^t \Omega^{-1} - \Omega^{-1} \Omega^t Q \rangle = -Ntr(\omega_{kl}) \langle \gamma, N \rangle - N(N-1)tr(\omega_{kl}) \langle \gamma, N \rangle \tag{A.15}
\]

\[
+ 2N(N-1)(N-2) \langle \omega_{kl}, \omega \gamma, N \rangle + 2N(N-1) \langle \omega_{kl}, \omega \gamma, N \rangle
\]

\[
= 2N \langle \omega_{kl}, N \rangle + 2N(N-1) \langle \omega_{kl}, \omega \gamma \rangle - \frac{1}{2} tr(\omega_{kl}) \langle \omega_{kl}, \gamma, N \rangle + 2N(N-1)(N-2) \langle \omega^{kl}, \omega \gamma, \gamma, N \rangle
\]

[1] Y. M. Zhao and A. Arima, Phys. Rep. 545, 1 (2014).
[2] M. G. Mayer, Phys. Rev. 75, 1969 (1949).
[3] J. H. D. Jensen, et al., Naturwissenschaften 36, 155 (1949).
[4] F. Iachello and I. Talmi, Rev. Mod. Phys. 59, 339 (1987).
[5] Y. A. Luo, et al., Nucl. Phys. A 669, 101 (2000).
[6] Y. M. Zhao, et al., Phys. Rev. C 62, 014315 (2000).
[7] L. Y. Jia, et al., Phys. Rev. C 75, 034307 (2007).
[8] X. F. Meng, et al., Phys. Rev. C 77, 044304 (2008).
[9] G. A. Jones, et al., Phys. Rev. C 76, 054317 (2007).
[10] Z. Y. Xu, et al., Phys. Rev. C 79, 054315 (2009).
[11] Y. Lei, Z. Y. Xu, Y. M. Zhao, and A. Arima, Phys. Rev. C 80, 064316 (2009).
[12] Y. Lei, Z. Y. Xu, Y. M. Zhao, and A. Arima, Phys. Rev. C 82, 034303 (2010).
[13] Y. Lei, Y. M. Zhao, A. Arima, Phys. Rev. C 84, 044301 (2011).
[14] A. Dewald, et al., Phys. Rev. C 37, 289 (1988).
[15] S. Harissopulos, et al., Phys. Rev. C 52, 1796 (1995).
[16] P. Das, et al., Phys. Rev. C 53, 1009 (1996).
[17] K. Higashiyama, et al., Phys. Rev. C 67, 044305 (2003).
[18] Y. Lei and Z. Y. Xu, Phys. Rev. C 92, 014317 (2015).
[19] Y. Y. Cheng, Y. Lei, Y. M. Zhao, and A. Arima, Phys. Rev. C 92, 064320 (2015).
[20] K. Sugawara-Tanabe and A. Arima, Phys. Lett. B 110, 87 (1982).
[21] S. Pittel and J. Dukelsky, Phys. Lett. B 128, 9 (1983).
[22] Y. Lei, G. J. Fu, and Y. M. Zhao, Phys. Rev. C 87, 044331 (2013).
[23] T. Mizusaki and T. Otsuka, Prog. Theo. Phys. Suppl. 125, 97 (1996).
[24] T. Otsuka, M. Honma, T. Mizusaki, N. Shimizu, and Y. Utsumo, Prog. Part. Nucl. Phys. 47, 319 (2001).
[25] http://www.netlib.org/blas/.
[26] C. G. Broyden, J. Inst. Math. Appl. 6, 76 (1970).
[27] R. Fletcher, Comp. J. 13, 317 (1970).
[28] D. Goldfarb, Math. Comp. 24, 23 (1970).
[29] D. F. Shanno, Math. Comp. 24, 647 (1970).
[30] J. Q. Chen, Nucl. Phys. A 626, 686 (1997).
[31] Y. M. Zhao, et al., Phys. Rev. C 62, 044304 (2000).
[32] J. A. White, S. E. Koonin, and D. J. Dean, Phys Rev C 61, 034303 (2000).
[33] I. Stetcu and C. W. Johnson, Phys. Rev. C 66, 034301 (2002); ibid. 67, 043315 (2013); ibid. 69, 024311 (2004).
[34] Y. Lei, Z. Y. Xu, Y. M. Zhao, and A. Arima, Phys. Rev. C 80, 064316 (2009).
[35] http://www.nndc.bnl.gov/ensdf/.
[36] D. R. Inglis, Phys. Rev. 96, 1059 (1954).