Shell-model-like approach based on cranking covariant density functional theory: bandcrossing and shape evolution in $^{60}$Fe

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Abstract

The shell-model-like approach is implemented to treat the cranking many-body Hamiltonian based on the covariant density functional theory including pairing correlations with exact particle number conservation. The self-consistency is achieved by iterating the single-particle occupation probabilities back to the densities and currents. As an example, the rotational structures observed in the neutron-rich nucleus $^{60}$Fe are investigated and analyzed. Without introducing any ad hoc parameters, the bandheads, the rotational spectra, and the relations between the angular momentum and rotational frequency for the positive parity band A, and negative parity bands B and C are well reproduced. The essential role of the pairing correlations is revealed. It is found that for band A, the bandcrossing is due to the change of the last two occupied neutrons from the $1f_{5/2}$ signature partners to the $1g_{9/2}$ signature partners. For the two negative parity signature partner bands B and C, the bandcrossings are due to the pseudo-crossing between the $1f_{7/2}, 5/2$ and the $1f_{5/2}, 1/2$ orbitals. Generally speaking, the deformation parameters $\beta$ for bands A, B, and C decrease with rotational frequency. For band A, the deformation jumps from $\beta \sim 0.19$ to $\beta \sim 0.29$ around the bandcrossing. In comparison with its signature partner band C, band B exhibits appreciable triaxial deformation.

Keywords: Shell-model-like approach, covariant density functional theory, cranking model, pairing correlations, collective rotation, bandcrossing, shape evolution, $^{60}$Fe

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I. INTRODUCTION

For the past decades, lots of novel phenomena with unexpected features in nuclear structure, including superdeformed rotational bands [1, 2], neutron halo [3, 4] and giant halo [5, 6], the disappearance and occurrence of magic numbers [8], magnetic and antimagnetic rotation [4, 12], chiral doublet bands [13, 14], and multiple chiral doublets (MχD) [17–19], have attracted worldwide attentions and challenged nuclear models aiming at a unified and microscopic interpretation of these novel phenomena.

Starting from an effective nucleon-nucleon interaction with Lorentz invariance, the covariant density functional theory (CDFT) naturally includes the spin-orbit coupling and has achieved great successes in describing many nuclear phenomena in stable and exotic nuclei of the whole nuclear chart [2, 3, 7, 13, 20]. Based on the same functional and without introducing any additional parameters, the CDFT can well describe the rotational excitations in nuclei by including the cranking terms [12, 21, 22]. Up to now, the cranking CDFT has been developed for the principal axis cranking (PAC) [23], the tilted axis cranking (TAC) [24, 25], and also for the aplanar TAC [24, 26]. With various versions of cranking CDFT, novel rotational phenomena including superdeformed rotational bands [23, 27, 28], magnetic [22, 24, 25, 29] and antimagnetic rotation [30, 31], linear cluster structure [32], and chiral doublet bands [24], have been investigated successfully.

Pairing correlations are essential to describe not only the nuclear ground state properties [24, 27, 34] but also the excited state properties [20, 37–38]. Within the mean-field approximation, the pairing correlations are usually treated by the Bardeen-Cooper-Schrieffer (BCS) approximation or Bogoliubov transformation [34]. However, the particle number is not conserved in the standard BCS and Bogoliubov approximations. The blocking effect, which is responsible for various odd-even differences in nuclear properties and important for low-lying excited states, can only be approximately considered. Another difficulty is the pairing correlation collapse with rotation [33]. Moreover, the BCS approximation can not be applied to the cranking model as the time-reversal symmetry is broken. Although these defects can be remedied by the particle number projection technique [34, 40–43], the calculation algorithm is complicated and the simplicity is lost [34].

Shell-model-like approach (SLAP) [44], or originally referred as particle number conserving (PNC) method [45], treats pairing correlations and blocking effects exactly by diagonal-
izing the many-body Hamiltonian in a many particle configuration (MPC) space with conserved particle number. Based on the phenomenological cranking Nilsson model, extensive applications for the odd-even differences in moments of inertia, identical bands, nuclear pairing phase transition, antimagnetic rotation, and high-$K$ rotational bands in the rare-earth and actinide nuclei, have been performed. Furthermore, the SLAP has been combined with CDFT, deformed Woods-Saxon potential, and the Skyrme density functional. Similar approaches to treat pairing correlations with conserved particle number can be found in Refs. Based on the CDFT, the SLAP has been firstly adopted to study the ground state properties and low-lying excited states for Ne isotopes. In Ref., the extension to include the temperature has been implemented to study the heat capacity.

In this paper, the SLAP is implemented to treat the cranking many-body Hamiltonian based on the CDFT including pairing correlations with exact particle number conservation, and is referred as cranking CDFT-SLAP. Our aim is to investigate the rotational excitation modes of superfluid nuclei in a fully microscopic, self-consistent, and particle number conserved manner. As an example, the rotational spectra in the neutron-rich nucleus $^{60}$Fe will be investigated with one of the most successful functionals PC-PK1. Being a key isotope in astrophysics and cosmic nucleosynthesis, the low-lying structure and rotational spectra in $^{60}$Fe have been investigated experimentally and theoretically with the projected shell model and the large-scale shell-model.

The paper is organized as follows. In Sec. the theoretical frameworks for the cranking CDFT and the SLAP are briefly presented. The numerical details are given in Sec. In Sec. the energy spectra and the relations between total angular momenta and rotational frequency for the three rotational bands in $^{60}$Fe calculated by the cranking CDFT-SLAP are presented and compared with the data. The bandcrossing mechanisms and shape evolutions in these rotational bands are discussed. A short summary is given in Sec. V.
II. THEORETICAL FRAMEWORK

A. Cranking covariant density functional theory

The effective Lagrangian density for the point-coupling covariant density functional is as follows \cite{31,79},

\[
\mathcal{L} = \mathcal{L}^{\text{free}} + \mathcal{L}^{4f} + \mathcal{L}^{\text{hot}} + \mathcal{L}^{\text{der}} + \mathcal{L}^{\text{em}} \\
\hat{\psi} (i\gamma_{\mu} \partial^{\mu} - m) \psi \\
- \frac{1}{2} \alpha_S (\hat{\psi} \gamma_{\mu} \psi)(\hat{\psi} \gamma_{\mu} \psi) - \frac{1}{2} \alpha_V (\hat{\psi} \gamma_{\mu} \psi)(\hat{\psi} \gamma_{\mu} \psi) \\
- \frac{1}{3} \beta_S (\hat{\psi} \psi)^3 - \frac{1}{4} \gamma_S (\hat{\psi} \psi)^4 - \frac{1}{4} \gamma_V [(\hat{\psi} \gamma_{\mu} \psi)(\hat{\psi} \gamma_{\mu} \psi)]^2 \\
- \frac{1}{2} \delta_S \partial_{\mu} (\hat{\psi} \psi) \partial^{\nu} (\hat{\psi} \psi) - \frac{1}{2} \delta_V \partial_{\mu} (\hat{\psi} \gamma_{\mu} \psi) \partial^{\nu} (\hat{\psi} \gamma_{\mu} \psi) - \frac{1}{2} \delta TV \partial_{\mu} (\hat{\psi} \gamma_{\mu} \psi) \partial^{\nu} (\hat{\psi} \gamma_{\mu} \psi) \\
- \frac{1}{4} F^{\mu\nu} F_{\mu\nu} - e \frac{1 - \tau_3}{2} \bar{\psi} \gamma^\mu \psi A_{\mu},
\]

(1)

which includes the free nucleon term \(\mathcal{L}^{\text{free}}\), the four-fermion point-coupling terms \(\mathcal{L}^{4f}\), the higher-order terms \(\mathcal{L}^{\text{hot}}\) responsible for the medium effects, the gradient terms \(\mathcal{L}^{\text{der}}\) simulating the effects of finite range, and the electro-magnetic interaction terms \(\mathcal{L}^{\text{em}}\).

To describe the nuclear rotation, the effective Lagrangian \(\mathcal{L}\) is transformed into a rotating frame with a constant rotational frequency \(\omega_x\) around the \(x\) axis \cite{21,27,80}. The equation of motion for the nucleons derived from the rotating Lagrangian is written as

\[
\hat{h}_0 \psi_{\mu} = (\hat{h}_{\text{s.p.}} + \hat{h}_c) \psi_{\mu} = \varepsilon_{\mu} \psi_{\mu},
\]

(2)

with

\[
\hat{h}_{\text{s.p.}} = \alpha \cdot (-i \nabla - V) + \beta (m + S) + V^0, \quad \hat{h}_c = -\omega_x \cdot \hat{j}_x,
\]

(3)

where \(\hat{j}_x = \hat{l}_x + \frac{1}{2} \Sigma_x\) is \(x\)-component of the total angular momentum of the nucleon spinors, and \(\varepsilon_{\mu}\) represents the single-particle Routhians for nucleons. The relativistic fields \(S(r)\) and \(V^\mu(r)\) have the form

\[
S(r) = \alpha_S \rho_S + \beta_S \rho_S^2 + \gamma_S \rho_S^3 + \delta_S \Delta \rho_S,
\]

\[
V^0(r) = \alpha_V \rho_V + \gamma_V \rho_V^3 + \delta_V \Delta \rho_V + \tau_3 \alpha TV \rho TV + \tau_3 \delta TV \Delta \rho TV + e \frac{1 - \tau_3}{2} A^0,
\]

\[
V(r) = \alpha_V \hat{j}_V + \gamma_V (\hat{j}_V)^3 + \delta_V \Delta \hat{j}_V + \tau_3 \alpha TV \hat{j} TV + \tau_3 \delta TV \Delta \hat{j} TV + e \frac{1 - \tau_3}{2} A,
\]

(4)
with $\rho$ and $j$ respectively represent the local densities and currents,

$$
\rho_S(r) = \sum_\mu n_\mu \bar{\psi}_\mu(r) \psi_\mu(r),
$$

$$
\rho_V(r) = \sum_\mu n_\mu \bar{\psi}_\mu(r) \psi_\mu(r),
$$

$$
\rho_{TV}(r) = \sum_\mu n_\mu \bar{\psi}_\mu(r) \tau_3 \psi_\mu(r),
$$

$$
\rho_{c}(r) = \sum_\mu n_\mu \bar{\psi}_\mu(r) \left(1 - \frac{\tau_3}{2}\right) \psi_\mu(r),
$$

(5)

in which $n_\mu$ is the occupation probability for each state $\mu$. The sums are taken over the states with positive energies only, i.e., the contributions of the negative-energy states are neglected (no-sea approximation). It is noted that the spatial components of the electro-magnetic vector potential $A$ are neglected since their contributions are extremely small.

After solving the equation of motion (2) self-consistently, the total energy of the system in the laboratory is obtained as,

$$
E_{\text{tot}} = E_{\text{kin}} + E_{\text{int}} + E_{\text{cou}} + E_{\text{c.m.}},
$$

(6)

with the energies of kinetic part,

$$
E_{\text{kin}} = \int d^3r \sum_\mu n_\mu \bar{\psi}_\mu(r) \left[ \alpha \cdot p + \beta m \right] \psi_\mu,
$$

(7)

the interaction part,

$$
E_{\text{int}} = \int d^3r \left\{ \frac{1}{2} \alpha_S \rho_S^2 + \frac{1}{3} \beta_S \rho_S^3 + \frac{1}{4} \gamma_S \rho_S^4 + \frac{1}{2} \delta_S \rho_S \Delta \rho_S
\right. \left. + \frac{1}{2} \alpha_V \left( \rho_V^2 - j \cdot j \right) + \frac{1}{2} \alpha_{TV} \left( \rho_{TV}^2 - j_{TV} \cdot j_{TV} \right)
\right.
\left. + \frac{1}{4} \gamma_V \left( \rho_V^2 - j \cdot j \right)^2 + \frac{1}{2} \delta_V \left( \rho_V \Delta \rho_V - j \Delta j \right)
\right.
\left. + \frac{1}{2} \delta_{TV} \left( \rho_{TV} \Delta \rho_{TV} - j_{TV} \Delta j_{TV} \right) \right\},
$$

(8)

the electro-magnetic part,

$$
E_{\text{cou}} = \int d^3r \frac{1}{2} e A_0 \rho_c,
$$

(9)
and the center-of-mass (c.m.) correction part,
\[ E_{\text{c.m.}} = -\frac{\langle \hat{P}_{\text{c.m.}}^2 \rangle}{2mA}, \tag{10} \]
with the mass number \( A \) and the total momentum in the center-of-mass frame \( \hat{P}_{\text{c.m.}} = \sum_i \hat{p}_i \).

The Dirac equation (2) can be solved by expanding the nucleon spinors in a complete set of basis states. In the present work, a three-dimensional harmonic oscillator (3DHO) basis in Cartesian coordinates \([24, 81–84]\) with good signature quantum number is adopted,

\[ \Phi_{\xi+}(r, s) = \langle r, s | \xi \alpha = + \rangle = \phi_{n_x} \phi_{n_y} \phi_{n_z} \frac{i^{n_y}}{\sqrt{2}} (-1)^{n_z+1} \left( \begin{array}{c} 1 \\ (-1)^{n_y+n_z} \end{array} \right), \tag{11} \]

\[ \Phi_{\xi-}(r, s) = \langle r, s | \xi \alpha = - \rangle = \phi_{n_x} \phi_{n_y} \phi_{n_z} \frac{i^{n_y}}{\sqrt{2}} \left( \begin{array}{c} 1 \\ (-1)^{n_y+n_z+1} \end{array} \right), \tag{12} \]

which correspond to the eigenfunctions of the signature operation with the positive (\( \alpha = +1/2 \)) and negative (\( \alpha = -1/2 \)) eigenvalues, respectively. The \( n_x, n_y \) and \( n_z \) are the harmonic oscillator quantum numbers in \( x, y, \) and \( z \) directions and \( \phi_{n_x}, \phi_{n_y} \) and \( \phi_{n_z} \) are the corresponding eigenstates. The phase factor \( i^{n_y} \) is added in order to get real matrix elements for the Dirac equation \([12]\). Furthermore, under the time-reversal operation \( \hat{T} = -i\sigma_y \hat{K} \), this 3DHO basis fulfills the following properties,

\[ \hat{T} \Phi_{\xi+}(r, s) = \Phi_{\xi-}(r, s), \quad \hat{T} \Phi_{\xi-}(r, s) = -\Phi_{\xi+}(r, s). \tag{13} \]

It means that under a proper phase factor, the \( \Phi_{\xi+} \) and \( \Phi_{\xi-} \) are a pair of time-reversal states with the same quantum numbers \( n_x, n_y \) and \( n_z \).

### B. Shell-model-like approach

The cranking many-body Hamiltonian with pairing correlations reads,

\[ \hat{H} = \hat{H}_0 + \hat{H}_{\text{pair}}. \tag{14} \]

The one-body Hamiltonian \( \hat{H}_0 = \sum \hat{h}_0 \) with \( \hat{h}_0 \) given in Eq. (4). The monopole pairing Hamiltonian \( \hat{H}_{\text{pair}} \) is used

\[ \hat{H}_{\text{pair}} = -G \sum_{\xi, \eta > 0} \beta_\xi^\dagger \beta_\eta^\dagger \beta_\xi \beta_\eta, \tag{15} \]
where $G$ is the effective pairing strength, $\tilde{\xi}$ ($\tilde{\eta}$) labels the time-reversal state of $\xi$ ($\eta$), and $\xi \neq \eta$ means that the self-scattering for the nucleon pairs is forbidden \cite{14}.

The one-body Hamiltonian $\hat{H}_0$ in the 3DHO basis \cite{11}-\cite{12} can be written as

$$\hat{H}_0 = \sum_{\xi\eta,\alpha} h_{\xi\alpha,\eta\alpha} \hat{b}_{\xi\alpha}^\dagger \hat{b}_{\eta\alpha}.$$  \hspace{1cm} (16)

Here $h_{\xi\alpha,\eta\alpha}$ is the matrix element of $\hat{h}_0$ between states $|\xi\alpha\rangle$ and $|\eta\alpha\rangle$. Accordingly, the pairing Hamiltonian $\hat{H}_{\text{pair}}$ in the 3DHO basis can be written as

$$\hat{H}_{\text{pair}} = -G \sum_{\xi\eta>0} \hat{b}_{\xi+\eta}^\dagger \hat{b}_{\xi-\eta} - \hat{b}_{\eta+\eta}^\dagger.$$  \hspace{1cm} (17)

The idea of SLAP is to diagonalize the many-body Hamiltonian in a properly truncated MPC space with exact particle number \cite{15}. One can diagonalize the cranking many-body Hamiltonian \cite{14} in the MPC space constructed from the single-particle states either in the CDFT or in the cranking CDFT. The latter is expected to achieve the same accuracy with smaller MPC space.

Diagonalizing the one-body Hamiltonian $\hat{H}_0$ \cite{14} in the basis $|\xi\alpha\rangle$ \cite{11}-\cite{12}, one can obtain the single-particle Routhian $\varepsilon_{\mu\alpha}$ and the corresponding eigenstate $|\mu\alpha\rangle$ for each level $\mu$ with the signature $\alpha$, namely,

$$\hat{H}_0 = \sum_{\mu\alpha} \varepsilon_{\mu\alpha} \hat{b}_{\mu\alpha}^\dagger \hat{b}_{\mu\alpha}, \quad |\mu\alpha\rangle = \sum_{\xi} C_{\mu\xi}(\alpha) |\xi\alpha\rangle.$$  \hspace{1cm} (18)

From the real expansion coefficient $C_{\mu\xi}(\alpha)$, the transformation between the operators $\hat{b}_{\mu\alpha}^\dagger$ and $\hat{b}_{\xi\alpha}^\dagger$ can be expressed as,

$$\hat{b}_{\mu\alpha}^\dagger = \sum_{\xi} C_{\mu\xi}(\alpha) \hat{b}_{\xi\alpha}^\dagger, \quad \hat{b}_{\xi\alpha}^\dagger = \sum_{\mu} C_{\mu\xi}(\alpha) \hat{b}_{\mu\alpha}^\dagger.$$  \hspace{1cm} (19)

In the $|\mu\alpha\rangle$ basis, the pairing Hamiltonian $\hat{H}_{\text{pair}}$ can be written as

$$\hat{H}_{\text{pair}} = -G \sum_{\mu\alpha\nu\nu'} \sum_{\xi,\eta>0} C_{\mu\xi}(+) C_{\nu\eta'}(+) C_{\nu\eta'}(-) C_{\nu\eta}(+) \hat{b}_{\mu+\nu}^\dagger \hat{b}_{\nu+\nu'}^\dagger \hat{b}_{\nu-\eta} \hat{b}_{\eta+\eta'}.$$  \hspace{1cm} (20)

From the single-particle Routhian $\varepsilon_{\mu\alpha}$ and the corresponding eigenstate $|\mu\alpha\rangle$ (briefly denoted by $|\mu\rangle$), the MPC $|i\rangle$ for an $n$-particle system can be constructed as \cite{85}

$$|i\rangle = |\mu_1\mu_2 \cdots \mu_n\rangle = \hat{b}_{\mu_1}^\dagger \hat{b}_{\mu_2}^\dagger \cdots \hat{b}_{\mu_n}^\dagger |0\rangle.$$  \hspace{1cm} (21)
The parity $\pi$, signature $\alpha$, and the corresponding configuration energy for each MPC are obtained from the occupied single-particle states.

The eigenstates for the cranking many-body Hamiltonian are obtained by diagonalization in the MPC space,

$$|\Psi\rangle = \sum_i C_i |i\rangle,$$

with $C_i$ the expanding coefficients.

The occupation probability $n_\mu$ for state $\mu$ is,

$$n_\mu = \sum_i |C_i|^2 P_{i\mu}, \quad P_{i\mu} = \begin{cases} 1, & |i\rangle \text{ contains } |\mu\rangle, \\ 0, & \text{otherwise}. \end{cases}$$

The occupation probabilities will be iterated back into the densities and currents in Eq. (5) to achieve self-consistency.

It is noted that, for the total energy in CDFT (6), the pairing energy due to the pairing correlations should be taken into account, $E_{\text{pair}} = \langle \Psi | \hat{H}_{\text{pair}} | \Psi \rangle$.

### III. NUMERICAL DETAILS

As mentioned before, the cranking many-body Hamiltonian (14) can be diagonalized in the MPC space constructed from the single-particle states either in the CDFT or in the cranking CDFT. The latter is expected to achieve the same accuracy with smaller MPC space.

In the following, the validity for diagonalizing the cranking many-body Hamiltonian (14) in MPC space constructed from the single-particle states in the cranking CDFT, namely cranking CDFT-SLAP, will be checked.

In the present cranking CDFT-SLAP calculations for $^{60}\text{Fe}$, the point-coupling density functional PC-PK1 [14] is used in the particle-hole channel and the monopole pairing interaction is adopted in the particle-particle channel. The equation of motion (2) is solved by expanding the Dirac spinor in terms of the three dimensional harmonic oscillator basis (11)-(12) with 10 major shells. For both neutron and proton, the dimensions of the MPC space are chosen as 800, which correspond to the energy cutoffs $E_c \approx 12.1$ and $\approx 18.5$ MeV, respectively. The effective pairing strengths are 0.8 MeV for both neutron and proton by
FIG. 1: (Color online) The neutron single-particle Routhian (a) and the alignment along the rotational axis $J_x$ (b) as functions of the rotational frequency in $^{60}\text{Fe}$ calculated by the cranking CDFT-SLAP with PC-PK1 [79], in comparison with the TAC-CDFT [25] calculations with tilted angle $\theta = 0^\circ$.

reproducing the experimental odd-even mass differences. Increasing the number of major shells from 10 to 12, the change of the total energy is within 0.1%. Increasing the dimension of the MPC space from 800 to 1200 and adjusting the effective pairing strength accordingly, the change of the total energy is within 0.1%. In the present calculation, there is no free parameter.

The validity for cranking CDFT-SLAP at the rotational frequency $\hbar \omega = 0.0$ MeV is confirmed by reproducing the results in Ref. [44], indicating that the pairing correlations have been taken into account correctly.

The validity for cranking CDFT-SLAP is also checked against the TAC-CDFT [25] calculation with the pairing correlations switching off. The neutron single-particle Routhian
and the alignment along the rotational axis $J_x = \langle \Psi | \hat{J}_x | \Psi \rangle$ as functions of the rotational frequency in $^{60}$Fe calculated by the cranking CDFT-SLAP are shown in Fig. 1, in comparison with the TAC-CDFT [25] calculations with tilted angle $\theta = 0^\circ$. Satisfactory agreement is found with the differences less than $10^{-4}$ MeV for the neutron single-particle Routhian and $10^{-4}\hbar$ for $J_x$.

IV. RESULTS AND DISCUSSION

Three rotational bands of the neutron-rich nucleus $^{60}$Fe have been observed in Ref. [76], including the yrast band with positive parity (labeled as band A) and two negative-parity signature partner bands with similar intensity starting from $6^-$ and $5^-$ states (labeled as bands B and C), respectively. As both parity and signature are good quantum numbers, the cranking many-body Hamiltonian (14) can be diagonalized in the corresponding MPC space. The yrast bands thus obtained for different parity and signature are compared with the observed bands A, B and C.

A. Energy spectra and $I - \omega$ relations

At a given rotational frequency, the eigenstate $|\Psi\rangle$ of the cranking many-body Hamiltonian (14) can be obtained by diagonalization in the MPC space. By adding the pairing energy $E_{\text{pair}} = \langle \Psi | \hat{H}_{\text{pair}} | \Psi \rangle$ to Eq. (6), the total energy of the system can be obtained. The corresponding spin $I$ can be obtained through $J_x = \langle \Psi | \hat{J}_x | \Psi \rangle = \sqrt{I(I+1)}$.

In Fig. 2, the total energies and the rotational frequencies are shown as functions of the spin for the positive parity band A, and negative parity signature partner bands B and C in $^{60}$Fe calculated by the cranking CDFT-SLAP with and without pairing correlations, in comparison with the available data.

In Figs. 2(a)-2(b), the cranking CDFT-SLAP calculations well reproduce the energy spectra for bands A, B and C without introducing any ad hoc parameters. Switching off the pairing correlations, the deviations appear for the low-spin regions, in particular for band A.

In Figs. 2(c)-2(d), the cranking CDFT-SLAP calculations well reproduce the $I - \omega$ relations including the bandcrossings for bands A, B and C. Switching off the pairing correla-
FIG. 2: (Color online) The total energies (a)-(b) and the rotational frequencies (c)-(d) as functions of the spin for the positive parity band A, and negative parity signature partner bands B and C in $^{60}$Fe calculated by the cranking CDFT-SLAP with and without pairing, in comparison with the data available $^{76}$. 

In Fig. 3, the deviations appear for the low-spin region for band A.

In Fig. 3, the pairing energies as functions of the rotational frequency for neutron and proton are shown for the positive parity band A, and negative parity signature partner bands B and C. Generally, the pairing energies decrease with rotational frequency, but without pairing correlation collapse. This is one of advantages of the SLAP.

For neutron, as seen in Fig. 3(a), the pairing energy in band A changes rapidly from \( \sim -5.0 \) MeV near the bandhead to \( \sim -1.5 \) MeV at \( \hbar \omega \approx 0.75 \) MeV, where the bandcrossing occurs. After bandcrossing, it changes similarly as bands B and C. In comparison with band A, the pairing energies in bands B and C are relatively small because the neutron pair in the 1$f_{5/2}$, 3/2 orbitals is broken (see in the following).

For proton, as seen in Fig. 3(b), the pairing energies change smoothly and similarly as functions of rotational frequency for bands A, B and C, which suggest that the proton configurations are the same. In comparison with the neutron, the suppressed pairing correlations

\[ \text{Spin I [\hbar]} \]

\[ \text{[c]} \]

\[ \text{[d]} \]

\[ \text{[e]} \]

\[ \text{[f]} \]
FIG. 3: (Color online) The pairing energies as functions of the rotational frequency for neutron (a) and proton (b) in the positive parity band A, and negative parity signature partner bands B and C.

for proton are due to the lower level density (see in the following).

The excellent agreements with the observed energy spectra and $I - \omega$ relations indicate that the cranking CDFT-SLAP correctly treats the pairing correlations and mean-field involved. From the calculations, one can pin down the corresponding configurations and examine the mechanism for bandcrossing.

B. Single-particle Routhians

To explore the mechanism of the observed bandcrossings, in Figs. 4 and 5, the single-particle Routhians as functions of the rotational frequency for bands A and B are shown.

As shown in Fig. 4(a), the occupied neutron orbitals for band A are changed around $\hbar \omega \approx 0.75 \text{ MeV}$. A discontinuity is observed in the neutron single-particle Routhians. Using the single-particle level tracking technique \cite{15}, the levels with the largest overlap ($> 0.9$) before and after the discontinuity are connected. It is found that the last two occupied neutrons change from the $1f_{5/2}$ signature partners to the $1g_{9/2}$ signature partners. The
FIG. 4: (Color online) The neutron (a) and proton (d) single-particle Routhians as functions of the rotational frequency for band A in $^{60}$Fe. Each orbital is labeled by the corresponding spherical quantum number of its main component. The positive (negative) parity levels are denoted by red (blue) lines. The signature $\alpha = +1/2 (-1/2)$ levels are denoted by solid (dash) lines. The solid circles denote the occupied orbitals, and the corresponding occupation probabilities $n_\mu$ are given in the right two columns.

occupation probabilities of the two $1g_{9/2}$ signature partners change from less than $10^{-1}$ at $\hbar \omega = 0.6$ MeV (c.f. Fig. 4(b)) to nearly 1 at $\hbar \omega = 1.2$ MeV (c.f. Fig. 4(c)). This configuration change for band A results from the rapid decrease of the neutron $1g_{9/2}$ orbitals with rotational frequency. For proton in band A, as shown in Figs. 4(d)-4(f), the occupation probabilities change smoothly. The discontinuity in the proton single-particle Routhians results from the change of the mean-field due to the neutron bandcrossing around $\hbar \omega \approx 0.75$ MeV. Hence, the configuration for band A after bandcrossing can be assigned as $\nu(1g_{9/2})^2(1f_{5/2})^{-2}$, which is in consistent with the assignment by the shell model $^{76}$ and the projected shell model $^{77}$.

For neutron in band B, as shown in Figs. 5(a)-5(c), the occupation probabilities change smoothly, and the neutron configuration can be assigned as $\nu(g_{9/2})^1(1f_{5/2})^{-1}$. For proton
in band B, as shown in Figs. 5(d) - 5(f), a pseudo-crossing is seen between the 1\(f_7/2\), 5/2 and the 1\(f_5/2\), 1/2 orbitals at \(\hbar \omega \approx 1.1\) MeV. The occupation probability of the proton 1\(f_5/2\), 1/2 orbital change from about \(10^{-2}\) to nearly 1, while that of the 1\(f_7/2\), 5/2 changes from nearly 1 to less than \(10^{-2}\).

As band C is the signature partner of band B, its detailed discussions of the neutron and proton single-particle Routhians and occupation probabilities are not shown here.

C. Angular momentum components

In the present fully self-consistent and microscopic cranking CDFT-SLAP calculation, the angular momentum can be calculated from the single neutron and proton orbitals. In Fig. 6, the contributions from the neutron and proton 1\(g_9/2\), (\(fp\)) and \(N/Z = 20\) shells to the angular momentum \(J_x\) for bands A, B and C are shown.

For all bands, both the \(N = 20\) and \(Z = 20\) shells do not contribute (core \(^{40}\)Ca is inert), and only nucleons in the (\(fp\)) shells and 1\(g_9/2\) orbitals contribute.
FIG. 6: (Color online) The contributions from the neutron and proton $1g_{9/2}$, ($fp$) and $N/Z = 20$ shells to the angular momentum $J_x$ as functions of the rotational frequency for the positive parity band A (a)-(b), and negative parity signature partner bands B (c)-(d) and C (e)-(f).

For neutron in band A, as shown in Fig. 6(a), the contributions from the ($fp$) shells change smoothly. After bandcrossing at $\hbar \omega \approx 0.75$ MeV, the contributions from the $1g_{9/2}$ orbitals are switched on, which produce a dramatic change around $6\hbar$. For proton, as shown in Fig. 6(b), the contributions are mainly from the ($fp$) shells, which have a kink around bandcrossing but change smoothly before and after.

For neutron in band B, as shown in Fig. 6(c), the contributions from the ($fp$) shells change smoothly. In contrast, the contribution from the $1g_{9/2}$ orbital keeps nearly unchanged ($\sim 4\hbar$) due to its high-$j$ low-$\Omega$ character. For proton, as shown in Fig. 6(d), the contributions from the ($fp$) shells increase smoothly with the rotational frequency but much faster after $\hbar \omega = 1.1$ MeV. This faster increase is due to the pseudo-crossing between the orbitals $1f_{7/2}$, $5/2$ and $1f_{5/2}$, $1/2$, as shown in Fig. 5(b).

For neutron and proton in band C, as shown in Figs. 6(e) and 6(f), the contributions of the angular momenta can be explained similarly as its signature partner band B.
FIG. 7: (Color online) The total Routhian surfaces for the positive parity band A (upper panels) at \( \hbar \omega = 0.0, 0.4, 0.8 \) and 1.2 MeV, and negative parity bands B (middle panels) and C (lower panels) at \( \hbar \omega = 0.4, 0.8 \) and 1.2 MeV. The red dot in the energy surface denotes the minimum. The energy difference between the neighboring contour lines is 0.5 MeV. The evolution of the deformation parameters \( \beta \) and \( \gamma \) with the rotational frequency are shown in the right column. For band A, the configurations before and after the bandcrossing are denoted as config.1 and config.2, respectively.

D. Shape evolution with rotation

To investigate the shape evolution with rotation in \( ^{60}\text{Fe} \), the total Routhian surfaces (TRSs) for the positive parity band A (upper panels) at \( \hbar \omega = 0.0, 0.4, 0.8 \) and 1.2 MeV, and negative parity signature partner bands B (middle panels) and C (lower panels) at \( \hbar \omega = 0.4, 0.8 \) and 1.2 MeV are shown in Fig. 7. The evolution of the deformation parameters \( \beta \) and \( \gamma \) with the rotational frequency are shown in the right column. For band A, the configurations before and after the bandcrossing are denoted as config.1 and config.2, respectively.
For band A, as mentioned before, the bandcrossing occurs at $\hbar \omega \approx 0.75$ MeV. Before the bandcrossing, the deformation parameters $(\beta, \gamma)$ of the TRS minimum at $\hbar \omega = 0.0$ MeV are around $(0.21, 0^\circ)$. With the increase of the rotational frequency, the deformation parameter $\beta$ decreases but the potential becomes more rigid. After the bandcrossing, the deformation parameters of the TRS minimum at $\hbar \omega = 0.8$ MeV are around $(0.29, 0^\circ)$. The dramatic change of the $\beta$ results from the deformation driving effect of the neutron $1g_{9/2}$ orbital. With the increase of the rotational frequency, the deformation parameter $\beta$ decreases but $\gamma$ increases. The potential becomes more rigid with $\beta$ but softer with $\gamma$. The deformation parameters of the TRS minimum at $\hbar \omega = 1.4$ MeV are around $(0.23, 12^\circ)$.

For band B, the deformation parameters of the TRS minimum at $\hbar \omega = 0.4$ MeV are around $(0.27, 12^\circ)$. With the increase of the rotational frequency, the deformation parameter $\beta$ decreases but $\gamma$ increases, and the potential becomes softer. The deformation parameters of the TRS minimum at $\hbar \omega = 1.2$ MeV are around $(0.21, 18^\circ)$.

Although bands B and C are signature partner bands, there is no triaxial deformation in band C. With the increase of the rotational frequency, the deformation of the TRS minimum decreases from $\beta = 0.27$ at $\hbar \omega = 0.4$ MeV to $\beta = 0.19$ at $\hbar \omega = 1.2$ MeV.

V. SUMMARY

In summary, the shell-model-like approach is implemented to treat the cranking many-body Hamiltonian based on the covariant density functional theory including pairing correlations with exact particle number conservation, referred as cranking CDFT-SLAP. The self-consistency is achieved by iterating the single-particle occupation probabilities back to the densities and currents.

As an example, the rotational spectra observed in the neutron-rich nucleus $^{60}\text{Fe}$, including the positive parity band A and two negative parity signature partner bands B and C, are investigated and analyzed. Without introducing any ad hoc parameters, the bandheads, the rotational spectra, and the relations between the angular momentum and rotational frequency for bands A, B, and C are well reproduced. It is found that pairing correlations are important to describe these quantities, especially for the low-spin part. By examining the single-particle Routhians, the occupation probabilities and the contributions from the $1g_{9/2}$, $(f_p)$ and $N/Z = 20$ shells to the angular momentum, the mechanisms of the bandcrossings.
are analyzed and discussed in detail. It is found that for band A, the bandcrossing is due to the change of the last two occupied neutrons from the $1f_{5/2}$ signature partners to the $1g_{9/2}$ signature partners. For the two negative parity signature partner bands B and C, the bandcrossings are due to the pseudo-crossing between the $1f_{7/2}, 5/2$ and the $1f_{5/2}, 1/2$ orbitals. The shape evolutions with rotation are investigated from the total Routhian surfaces. For band A, the deformation parameter $\beta$ decreases with rotational frequency before and after the bandcrossing. A dramatic change of $\beta$ is observed around the bandcrossing at the frequency $\hbar \omega \approx 0.75$ MeV, which results from the deformation driving effect of the neutron $1g_{9/2}$ orbital. For band B, the deformation evolves from $(0.27, 12^\circ)$ at $\hbar \omega = 0.4$ MeV to $(0.21, 18^\circ)$ at $\hbar \omega = 1.2$ MeV. For band C, there is no triaxial deformation, and the deformation evolves from $\beta = 0.27$ at $\hbar \omega = 0.4$ MeV to $\beta = 0.19$ at $\hbar \omega = 1.2$ MeV.

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