Backbending and \( \gamma \) vibrations

J. Kvasil\(^1\) and R. G. Nazmitdinov\(^2,3\)

\(^1\)Institute of Particle and Nuclear Physics, Charles University, V. Holesovická 2, CZ-18000 Praha 8, Czech Republic

\(^2\)Departament de Física, Universitat de les Illes Balears, E-07122 Palma de Mallorca, Spain

\(^3\)Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, 141980 Dubna, Russia

We propose that the backbending phenomenon can be explained as a result of the disappearance of collective \( \gamma \)-vibrational mode in the rotating frame. Using a cranking + random phase approximation approach for the modified Nilsson potential + monopole pairing forces, we show that this mechanism is responsible for the backbending in \(^{156}\)Dy and \(^{158}\)Er, and obtain a good agreement between theoretical and experimental results.

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There is a general persuasion that the backbending is caused by the rotational alignment of angular momenta of a nucleon pair occupying a high-j intruder orbital near the Fermi surface. It is assumed that the alignment breaks a singlet Cooper pairing in this pair and leads to a sudden increase of the kinematical moment of inertia, \( \mathcal{J}^{(1)} = I/\Omega \) along the yrast level sequence as a function of a rotational frequency \( \Omega \) (cf Ref.\(^1\)). Indeed, in many cases this single-particle (quasiparticle) mechanism is supported by microscopic analysis in terms of various cranking Hartree-Fock-Bogoliubov calculations (cf Refs.\(^2,3,4\)). It should be noted, however, that the role of vibrational (collective) excitations in the backbending has never been studied.

It is well known that mean field description of finite Fermi systems could break spontaneously one of the symmetries of the exact Hamiltonian, the so-called spontaneously symmetry breaking (SSB) phenomenon. In fact, the mean field description of the backbending corresponds to the first-order phase transition. However, this concept is appropriate only in the limit of infinite number of particles. Obviously, for finite systems quantum fluctuations, beyond the mean field approach, are quite important. The random phase approximation (RPA) being an efficient tool to study these quantum fluctuations (vibrational and rotational excitations) provides also a consistent way to restore broken symmetries. Moreover, it separates the collective excitations associated with each broken symmetry as a spurious RPA mode and fixes the corresponding inertial parameter. In this paper we present the first self-consistent quantitative treatment of these ideas for rotating nuclei.\(^3\) We demonstrate that the backbending in \(^{156}\)Dy and \(^{158}\)Er can be explained as a result of vanishing one of the quadrupole vibrational modes in the rotating frame at a critical rotational frequency. Consequently, collective motion associated with this mode should describe rotational states of the nonaxial rotating system.

The practical application of the RPA for nonseparable effective forces such as the Gogny or Skyrme interactions in rotating nuclei requires too large configuration space and still is not-available. The RPA with separable multipole-multipole interaction based upon phenomenological cranking Nilsson or Saxon-Woods potentials with pairing forces gives a sufficiently good description of low-lying collective excitations in rotating nuclei (cf Refs.\(^3,4\)). Following this approach, which hereafter is called CRPA, we start with the cranking shell model (CSM) Hamiltonian in the form

\[
H_\Omega = H - \sum_{\tau=1}^3 \chi_\tau N_\tau - \Omega \hat{J}_z + H_{\text{int}}. \tag{1}
\]

The term \( H = H_N + H_{\text{add}} \) contains a Nilsson Hamiltonian \( H_N \) with three different oscillator frequencies \( \omega_i^2 = \omega_0(\beta_i, \gamma_i)^2 \left[ 1 - 2\beta_i \sqrt{\frac{\omega_0}{\omega_i}} \cos(\gamma_i - \frac{\pi}{4}) \right] \) (\( i = 1, 2, 3 \)) that determine quadrupole deformation parameters \( \gamma \) and \( \beta \) (cf Refs.\(^3,4\)). The frequencies are subject to the volume conservation constraint \( \omega_1^2 + \omega_2^2 + \omega_3^2 = \omega_0^2 \) (\( \hbar \omega_0 = 41 A^{-\frac{1}{3}} \) MeV) that models the nuclear incompressibility. In the cranking model with the standard Nilsson potential the value of the moment of inertia is largely overestimated due to the presence of the velocity dependent \( \bar{l}_z^2 \) term. This shortcoming can be overcome by introducing the additional term \( H_{\text{add}} = \sum_i h_{\text{add}}(i) \) with

\[
h_{\text{add}} = - \Omega m \omega_0 \kappa \left[ 2 \left( r^2 s_z - \vec{x} \cdot \vec{s} \right) \right] \tag{2}
\]

\[+ \mu \left( 2r^2 - \frac{\hbar}{m\omega_0} (N + \frac{3}{2}) \right) l_z \].

The term restores the local Galilean invariance of the Nilsson potential in the rotating frame and removes the spurious effects of the \( \bar{l}_z^2 \) term (see for details Ref.\(^7\)). Note that this basic recipe supersedes the fitting procedure of nuclear inertial properties used, for example, in Ref.\(^1\).

The interaction is taken in a separable form

\[
H_{\text{int}} = - \sum_\tau G_\tau \hat{P}_+^\tau \hat{P}_-^\tau - \frac{1}{2} \kappa_2 \left[ \sum_{\sigma,m} \hat{Q}_m^{(\sigma)} \hat{M}_m^{(+)} \right]. \tag{3}
\]

Here, \( \tau = \) neutrons or protons, \( \hat{P}_+^\tau = \sum_k c_k^+ c_k^\tau \) and \( c_k^\tau, c_k \) are creation and annihilation single-particle operators.
respectively. An index $k$ is labelling a complete set of the oscillator quantum numbers $|k\rangle = |N_i j m_j\rangle$ and the index $\tilde{k}$ denotes the time-conjugated state $|\tilde{k}\rangle$. We recall that the K quantum number (a projection of the angular momentum on the quantization axis) is not conserved in rotating non-axially deformed systems. However, the CSM Hamiltonian adheres to the $D_2$ spatial symmetry with respect to rotation by the angle $\pi$ around the rotational axis $x$. Consequently, all rotational states can be classified by the quantum number called signature $\sigma = \exp(-i\pi\alpha)$ leading to selection rules for the total angular momentum $I = \alpha + 2n$, $n = 0, \pm 1, \pm 2, \ldots$. In particular, in even-even nuclei the lowest rotational (yrast) band characterized by the positive signature quantum number $\sigma = 1 (\alpha = 0)$ consists of even spins only.

The quadrupole operators $\hat{Q}_m$ ($m = 0, 1, 2$) are defined by

$$\hat{Q}_m^{(\sigma)} = \frac{i^{2+m+(\sigma+3)/2}}{\sqrt{2(1 + \delta_m)}} \chi^2 \left( Y_{2m} + (-1)^{(\sigma+3)/2} Y_{2-m} \right). \quad (4)$$

The monopole interaction is defined by the positive signature operator $\hat{M}^{(+)} = r^2 Y_0$. Single-particle matrix elements of any one-body Hermitian operator $\hat{F}(P, Q, M)$ are determined by the signature, time-reversal and Hermitian conjugation properties of the operator (cf Ref [6]). All multipole expressions in terms of the double-stretched coordinates $\hat{q}_i = \frac{\hbar}{\mu} q_i$, ($q_i = x, y, z$). The effective interaction restores the rotational invariance of the Hamiltonian $\hat{H}$ in the limit of the harmonic oscillator potential $\hat{V}$. This is especially important in order to establish a relation between SSB of the rotating mean field and an appearance of the corresponding RPA spurious mode (cf Ref [12]). While a qualitative discussion about a relation between SSB effects and RPA spurious modes in non-rotating nuclei could be found in literature (cf Ref [1, 13], here we present the first realistic quantitative attempt to get a thorough insight into this relation in rotating nuclei. The self-consistent determination of the constants $G$ and $K_2$ will be discussed below.

Using the generalized Bogoliubov transformation for quasiparticles (for example, for the positive signature quasiparticle we have $\alpha_i^q = \sum_k U_{ki} c_k^+ c_k$ and the variational principle (see details in Ref [6]), we obtain the Hartree-Bogoliubov (HB) equations. The HB equations are solved using the "experimental" values of deformation parameters $\beta$ and $\gamma$ (see Fig [11]), obtained in Ref [14] as an input. These values are extracted from experimental data [14]. For the pairing field $\Delta_{kl} = -\delta_{kl} G_t (\bar{P}_r) = \delta_{kl} \Delta_r (\Omega)$ we assume a phenomenological dependence of the pairing gap $\Delta_r$ upon the rotational frequency $\Omega$

$$\Delta_r (\Omega) = \begin{cases} \Delta_r (0) \left[ 1 - \frac{1}{\mu} \left( \frac{\Omega}{\Omega_c} \right)^2 \right] & \text{for } \Omega < \Omega_c, \\ \Delta_r (0) \frac{1}{2} \left( \frac{\Omega}{\Omega_c} \right)^2 & \text{for } \Omega > \Omega_c, \end{cases} \quad (5)$$

introduced in Ref [14]. Here, $\Omega_c = 0.32, 0.33$ MeV is a rotational frequency where the first band crossing (which is approximately the same for protons and neutrons) occurs for $^{156}$Dy and $^{158}$Er, respectively. The values of pairing gaps $\Delta_r (0) = 0.857$ MeV, $\Delta_r (0) = 0.879$ MeV (for $^{156}$Dy) and $\Delta_r (0) = 0.874$ MeV, $\Delta_r (0) = 0.884$ MeV (for $^{158}$Er) are obtained from the odd-even mass difference (see also Ref [15]). The Nilsson parameters $\kappa$ and $\mu$ are taken from systematic analyses for all deformed nuclei [8]. In our calculations we include all shells up to $N = 8$ and consider $\Delta N = 2$ mixing. The configuration space exhausted 97% of energy weighted sum rule for quadrupole transitions.

It is enough to solve the HB equations only for the positive signature quasiparticle energies $\varepsilon_i$, since the negative signature eigenvalues $\bar{\varepsilon}_i$ and eigenvectors ($U_{ki}, V_{ki}$) are obtained from the positive ones. Thus, our quasiparticle operators are defined with respect to the yrast state $|\bar{\gamma}\rangle$ (the lowest HB state at given $\Omega$) which is our quasiparticle vacuum $\alpha_i|\bar{\gamma}\rangle = 0, \alpha_i|\bar{\gamma}\rangle = 0$.

In the limit of the harmonic oscillator, at the self-consistent energy minimum the expectation values of the operators $Q_0$ and $Q_2^{(+)}$ expressed in the double-stretched coordinates, Eqs. (4), are zeros

$$\langle Q_0 \rangle = \langle Q_2^{(+)} \rangle = 0 \quad (6)$$

In other words, the self-consistent residual interaction does not change the mean field equilibrium deformation. To check the self-consistency of the HB solutions, we calculate Eqs. (6) when all terms are included in the HB equations. First, we would like to stress that the "experimental" values of $\beta$ and $\gamma$ correspond, indeed, to the minimum of the total mean field (HB) energy. The variation of the deformation parameters $\beta$ and $\gamma$ around the "experimental" (equilibrium) values results in the increase of the HB energy. This minimum becomes very shallow, however, with the increase of the rotational frequency. Second, double-stretched quadrupole moments are approximately zero for all values of the equilibrium deformation parameters. A small deviation from the equilibrium space exhausted 97% of energy weighted sum rule for quadrupole transitions.

FIG. 1: (Color online) Equilibrium deformations in $\beta$-$\gamma$ plane as a function of the angular momentum $I = \langle J_z \rangle$ (in units of $\hbar$).
reproduce better the experimental data. Our equilibrium deformations are a result of the self-consistent solutions of the HB equations, whereas the authors of Ref.6 used fixed phenomenological inertial parameters.

To describe quantum oscillations around mean field solutions the boson-like operators \( b^+_{kl} = \alpha^+_k \alpha^+_l, b^+_{kl} = \alpha^+_k \alpha^+_l \) are used. The first equality introduces the positive signature boson, while the other two determine the negative signature ones. These two-quasiparticle operators are treated in the quasi-boson approximation (QBA) as an elementary bosons, i.e., all commutators between them are approximated by their expectation values with the uncorrelated HB vacuum. The corresponding commutation relations can be found in Ref.6. In this approximation any single-particle operator \( F \) can be expressed as \( \hat{F} = \langle F \rangle + \hat{F}^{(1)} + \hat{F}^{(2)} \) where the second and third terms are linear and bilinear order terms in the boson expansion. We recall that in the QBA one includes all second order terms into the boson Hamiltonian such that \( \langle F - \langle F \rangle \rangle^2 = \hat{F}^{(1)} \hat{F}^{(2)} \). The positive and negative signature boson spaces are not mixed, since the corresponding operators commute and \( H_0 = H_0(\sigma = +) + H_0(\sigma = -) \).

The CRPA Hamiltonian is diagonalized by solving the equations of motion for each signature separately. As a result, we obtain the following determinant of the secular equations

\[
\mathcal{F}(\omega_\lambda) = \det (R - \frac{1}{2c}),
\]

which is the fifth and the second order for the positive and negative signature, respectively, and \( c = \kappa_2 \) or \( G_x \). The matrix elements \( R_{km}(\omega_\lambda) = \sum_\mu \zeta_{k\mu} \zeta_{m\mu} C^\mu_{km} / (\omega^2_\lambda - \omega^2_\mu) \) involve the coefficients \( C^\mu_{km} = \omega_\mu / \omega_\lambda \) for different combinations of matrix elements \( \zeta_{k\mu} \) (see details in Refs.6,7). The zeros of the function \( \mathcal{F}(\omega_\lambda) \) yield the CRPA eigenfrequencies \( \omega_\lambda \). Since the mean field violates the rotational invariance and particle number conservation law, among the CRPA eigenfrequencies there exist few spurious solutions. In this paper we focus our attention on the SSB effects related to the rotation, since the pairing can be treated in the same way.

Introducing the operator \( \Gamma^+ = (\hat{j}^{(1)}_x - i \hat{j}^{(2)}_x) / \sqrt{2} \langle J_x \rangle \) such that

\[
[H_0(\sigma = +), \Gamma^+] = \Omega \Gamma^+, \quad [\Gamma, \Gamma^+] = 1, \quad \Gamma = (\Gamma^+)^+ \quad (8)
\]

one is able to separate negative signature vibrational modes from the "spurious" solution at \( \omega_\lambda = \Omega \). Equations (8) describe a collective phonon that creates a collective rotation. This phonon is related to the symmetry broken by the external rotational field (the cranking term in Eq.11).

The other spurious solutions are associated with the rotation around the x axis and the particle number conservation law,

\[
[H_0, \hat{J}_x] = [H_0, \hat{N}_e] = 0. \quad (9)
\]

The mode associated with the rotation about the x axis allows one to determine the Thouless-Valatin moment of inertia \( J_{TV} \) using the positive signature term of the full Hamiltonian

\[
[H_\Omega(\sigma = +), i \hat{\Phi}] = \frac{\hat{J}_x}{J_{TV}}, \quad [\hat{\Phi}, \hat{J}_x] = i. \quad (10)
\]

Here the angle operator \( \hat{\Phi} \) is the canonical partner of the angular momentum operator \( \hat{J}_x \). A similar procedure can be applied for the second spurious mode in Eqs. (9) to obtain the mass parameters for neutron or protons 13,19.

It is important to hold a self-consistency at the CRPA level as well as at the mean field. In the harmonic oscillator limit the self-consistent constant, \( \kappa_2 = \frac{4 \pi m \omega_\lambda^2}{\hbar} \), warrants the fulfillment all conservation laws in the CRPA for rotating nuclei 12. Therefore, in our realistic calculations we define the constants from the requirement of the fulfillment of the conservation laws, Eqs. (9), and a separation of the rotational mode from the vibrational ones, Eqs. (8). It was proved in Ref.12 for the self-consistent model, which can be solved exactly, that the dynamical \( \hat{J}_{HB}^{(2)} \) and the Thouless-Valatin \( J_{TV} \) moments of inertia must coincide, if one found a self-consistent mean field minimum and spurious solutions are separated from the physical ones. Our results (see Fig.2) demonstrate a good self-consistency between the mean field and the CRPA calculations, indeed.

![FIG. 2: The rotational dependence of the dynamical \( \hat{J}_{HB}^{(2)} = -d^2 E_{HB}/d\Omega^2 = d(\hat{J}_x)/d\Omega \) (a dash line) and the Thouless-Valatin \( J_{TV} \) moments of inertia (a solid line). Here, \( E_{HB} \) is a mean field value of the full Hamiltonian.](image)

To analyze the low-lying excited states we construct the Routhian function for each rotational band \( (\nu = yrst, \beta, \gamma, \ldots) \)

\[
R_\nu(\Omega) = E_\nu(\Omega) - \Omega L(\Omega)
\]

and define the experimental excitation energy in the rotating frame \( \omega_\nu(\Omega) = R_\nu(\Omega) - R_yr(\Omega) \) 21. This energy can be directly compared with the corresponding solutions \( h\omega_\lambda \) of the CRPA secular equations. The experimental Routhians \( R_\nu \) are obtained from experimental data 21.
The results demonstrate a good agreement between theory and experiment (see Fig.3). The lowest collective \( \gamma \) vibrational frequency for the positive signature states (even spins) becomes zero at \( \hbar \Omega_{cr} \approx 0.324 \) and 0.33 MeV for \(^{156}\text{Dy}\) and \(^{158}\text{Er}\), respectively. As discussed above, near the rotational frequency \( \Omega_{cr} \) the backbending occurs in the considered cases.

In order to understand this correlation, let us consider an axially deformed system, defined by the Hamiltonian \( \hat{H} \) in the laboratory frame, that rotates about a symmetry axis \( z \) with a rotational frequency \( \Omega \). The angular momentum is a good quantum number and, consequently, \( [\hat{J}_z, \hat{O}_K^j] = \hat{K}\hat{O}_K^j \). Here, the CRPA phonon \( \hat{O}_K^j \) describes the vibrational state with \( K \) being the value of the angular momentum carried by the phonons \( \hat{O}_K^j \) along the symmetry axis, \( z \) axis. Thus, one obtains

\[
[H, \hat{O}_K^j] = [\hat{H} - \Omega \hat{J}_z, \hat{O}_K^j] = (\hat{\omega}_K - K\Omega)\hat{O}_K^j \equiv \omega_K\hat{O}_K^j.
\]

This equation implies that at the rotational frequency \( \Omega_{cr} = \hat{\omega}_K/K \) one of the CRPA frequency \( \omega_K \) vanishes in the rotating frame (see discussion in Refs.22, 23). At this frequency we could expect the SSB effect of the rotating mean field due to the appearance of the Goldstone boson related to the multipole-multipole forces with quantum number \( K \). For an axially deformed system one obtains the breaking of the axial symmetry, since the lowest critical frequency corresponds to \( \gamma \) vibrations with \( K = 2 \) 22, 23. In contrast to nonrotating case 13, the RPA does not break down at the bifurcation point, since in the laboratory system the corresponding vibration still persists.

**FIG. 3:** (Color online) The excitation energies in the rotating frame \( \omega_\gamma (\Omega) \) for the positive signature \( \gamma \) (top panel) and \( \beta \) vibrational (bottom panel) states. The results of calculations are connected by a solid line. The lowest two-quasiparticle states shown at the upper panel are connected by a dash line. The experimental values for different excitations are indicated by open circles connected by a thin line to guide eyes.

**FIG. 4:** The rotational dependence of the mean field value \( \langle J_z \rangle \) (in units \( \hbar \)) for \(^{156}\text{Dy}\) (left panel) and \(^{158}\text{Er}\) (right panel). The noncollective angular momentum is built by the alignment of the separate two-quasiparticle pairs till \( \Omega_{cr} \approx 0.32 \) (MeV) in both nuclei.

Guided by this analysis, we solve the HB equations with rotation about the symmetry axis \( z \) (the noncollective regime). Since the angular momentum of a quasiparticle state is conserved, the lowest two-quasiparticle configuration with the largest deformation aligned orbitals builds the total angular momentum of the system when it crosses the ground state configuration with zero angular momentum. The total angular momentum increases each time stepwise by an amount of angular momentum carried by a two-quasiparticle configuration that crosses the renewed ground state configuration. For \(^{156}\text{Dy}\) (see Fig.4) \( \langle J_z \rangle \) is zero for all rotational frequencies in the range of values \( 0 \leq \hbar \Omega \leq 0.275 \) MeV. At \( \hbar \Omega = 0.275 \) MeV the energy of the neutron two-quasiparticle state originating from the shells \( h9/2 \otimes f7/2 \) (for \( \Omega = \Delta = 0 \) it is the configuration built from the Nilsson states \( \frac{5}{2} \otimes \frac{7}{2} \)) goes to zero. The nuclear angular momentum is determined by the angular momentum of this two-quasiparticle state: \( \langle J_z \rangle = \frac{5}{2} + \frac{7}{2} = 8\hbar \). Note that one would expect the onset of the nonaxiality at this frequency, according to the quasiparticle picture. According to our results, at \( \hbar \Omega = 0.31 - 0.32 \) MeV the expectation value \( \langle J_z \rangle \) is increased stepwise by next four units. The system remains an axially deformed creating a state with \( \langle J_z \rangle = 12\hbar \). At \( \hbar \Omega_{cr} = 0.324 \) MeV the system acquires additional two units and the shape transition occurs to a nonaxially deformed shape. We recall that at this frequency \( \gamma \) vibrations of the positive signature carrying two units of the angular momentum vanish. Comparing the calculated value of the critical frequency with the experimental estimation \( \hbar \Omega_{cr} = h\hat{\omega}_K/\Delta = 0.691/2\,MeV \approx 0.345 \) MeV, one could find a good agreement between theory and experiment. As was mentioned above, the potential energy surface is very shallow at large rotational frequencies. In fact, the energy minima for a rotation around the axis \( z \) and the axis \( x \) are almost degenerate. The difference is about 15 keV near the critical rotational frequency.
At the bifurcation point a competition between the collective (around the axis $x$) and noncollective rotations breaks the axial symmetry and leads to nonaxial shapes.

For $^{158}\text{Er}$ the experimental critical value is expected at $\hbar\Omega_{cr} = \hbar\omega_{K=2} = 0.613/2$ MeV $\sim 0.306$ MeV. The angular momentum is zero up to the rotational frequency $\hbar\Omega = 0.272$ MeV. At this frequency the proton two-quasiparticle state originating from $h7/2 \otimes d5/2$ shells (for $\Omega = \Delta = 0$ this configuration is built from the Nilsson states $\frac{7}{2}[404] \otimes \frac{5}{2}[402]$) contributes to the value of the angular momentum $\frac{7}{2} = \frac{5}{2} = 6\hbar$. The system remains the axially deformed, getting another two units of the angular momentum, up to $\hbar\Omega_{cr} \approx 0.33$ MeV, where $\gamma$ vibrations of the positive signature are vanished in the rotating frame. Again, there is a tiny energy difference between the collective and noncollective rotations ($\sim 15$ keV). At this frequency the expectation value $\langle J_z \rangle$ is increased by two more units and for $\Omega > \Omega_{cr}$ the system is driven into the domain of triaxial shape.

According to the CRPA, the reduced transition probability between $\gamma$ (one-phonon) states of the positive signature $B(E2, \Delta I = 2) \sim |\langle Q_2^+(\Delta I = 2) \rangle|^2$ is of the same order of magnitude as the collective electric quadrupole transitions between yrast (vacuum) states. In fact, in both nuclei the $B(E2, \Delta I = 2)$ strength exceeds few tens of Weisskopf units. Detailed calculations of the transition probabilities are beyond the scope of the present paper and will be presented elsewhere.

Summarizing, for the first time the cranking HB and RPA equations are solved in a self-consistent manner. We obtain a good agreement with available experimental data for low-lying vibrational excitations at high spins in $^{156}\text{Dy}$ and $^{158}\text{Er}$. According to our analysis, the alignment decreases the pairing correlations and, consequently, the $\gamma$ vibrations are softening in axially deformed nuclei. We stress that the two-quasiparticle alignment does not create the backbending. Rotating around the axis which is perpendicular to the symmetry axis, we found that in $^{156}\text{Dy}$ and $^{158}\text{Er}$ the backbending occurs at the critical rotational frequency $\Omega_{cr} \approx \omega_{K=2}/2$ where $\omega_{K=2}$ is a $\gamma$ vibrational excitations in the laboratory frame at $\Omega = 0$. At this frequency the positive signature $\gamma$ vibrational excitations vanish in the rotating frame, i.e., $\omega_{K=2} = 0$. As a result, the nuclear mean field spontaneously breaks the axial symmetry and gives rise to nonaxially deformed shape in the rotating frame. Thus, the inclusion of quantum fluctuations around the mean field approach extending our understanding of the backbending phenomenon.

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