Microscopic Formulation of Interacting Boson Model for Rotational Nuclei

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We propose a novel formulation of the Interacting Boson Model (IBM) for rotational nuclei with axially-symmetric strong deformation. The intrinsic structure represented by the potential energy surface (PES) of a given multi-nucleon system has a certain similarity to that of the corresponding multi-boson system. Based on this feature, one can derive an appropriate boson Hamiltonian as already reported. This prescription, however, has a major difficulty in rotational spectra of strongly deformed nuclei: the bosonic moment of inertia is significantly smaller than the corresponding nucleonic one. We present that this difficulty originates in the difference between the rotational response of a nucleon system and that of the corresponding boson system, and could arise even if the PESs of the two systems were identical. We further suggest that the problem can be cured by implementing $L-L$ term into the IBM Hamiltonian, with coupling constant derived from the cranking approach of Skyrme mean-field models. The validity of the method is confirmed for rare-earth and actinoid nuclei, as their experimental rotational yrast bands are reproduced nicely.

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The atomic nucleus is a strongly interacting many-body quantal system which has collective properties resulting in various deformed shapes. If a nucleus is strongly deformed, it rotates, exhibiting characteristic rotational band structure with remarkable regularity. Such rotational motion can be viewed as a manifestation of symmetry restoration mechanism of Nambu, and has attracted much attention in nuclear physics from various viewpoints [1, 2].

The Interacting Boson Model (IBM) [3, 4] has been successful in phenomenological studies for describing low-lying quadrupole collective states of medium-heavy nuclei [5]. The major assumption of the IBM is to employ $L = 0^+$ ($s$) and $L = 2^+$ ($d$) bosons which reflect the collective $S$ and $D$ pairs of valence nucleons [5]. The microscopic foundation of the IBM has been studied extensively so as to derive an IBM Hamiltonian starting from nucleon degrees of freedom [6, 7]. A new approach to derive the IBM Hamiltonian has been presented recently [8]. In this approach, the potential energy surface (PES) with quadrupole degrees of freedom, obtained from the mean-field calculation with the Skyrme Energy Density Functional (EDF) [9, 10], is compared to the corresponding PES of IBM to obtain the parameters of IBM Hamiltonian. As a Skyrme EDF gives universal descriptions of various nuclear structures [2, 6, 9, 11], one can derive the IBM Hamiltonian basically for all situations in a unified way. This method turned out to be valid particularly for nuclei with weak to moderate quadrupole deformation, and has been practiced extensively [12]. When a nucleus is well deformed, however, the nucleonic rotational spectrum appears notably and systematically different from the corresponding bosonic one, being manifested by too small bosonic moment of inertia as compared to the corresponding fermionic one [8, 12].

This kind of difference has been known as a result of limited degrees of freedom, $s$ and $d$ bosons only, in many cases [13, 14]. In order to remedy this problem, another type of nucleon pairs, e.g., $L = 4^+$ ($G$) pair, and the corresponding boson image ($g$ boson) have been introduced, and their effects were renormalized into $sd$ boson sector, yielding IBM Hamiltonians consistent with phenomenological ones [6, 7, 13, 21]. In the mean time, the validity of IBM for rotational nuclei was analyzed in terms of the Nilsson model [22], coming up with the criticism that the $SD$-pair truncation may be far from sufficient for describing intrinsic states of strongly deformed nuclei, and this naturally casts a question on the applicability of the IBM to rotational nuclei in particular. While it has been reported that the $SD$-pair dominance holds to a good extent in intrinsic states of rotational nuclei [15, 23, 24], there has been no conclusive mapping procedure from nucleonic systems to IBM ones covering rotational nuclei. It is thus of much interest to revisit this issue with the newly proposed method of Ref. [8], looking for a prescription to cure the afore-mentioned problem of too small moment of inertia.

In the method of Ref. [8], we calculate the energies of nucleonic and bosonic intrinsic states representing various shapes, and obtain PESs. We then determine parameters of the IBM Hamiltonian so that the bosonic PES becomes similar to the nucleonic one [8]. These intrinsic states are at rest with rotational frequency $\omega = 0$. In this paper, we move on by one step further with non-zero rotational frequency $\omega \neq 0$. Actually we analyze the responses of the nucleonic and bosonic intrinsic states by rotational cranking with infinitesimal $\omega$. From such responses, one can extract the most important rotational correction to the IBM Hamiltonian.

The nucleon intrinsic state $|\phi_F\rangle$ is obtained from the Hartree-Fock plus BCS (HF+BCS) calculation. Skyrme SkM* interaction [26] is used throughout, while different
Skyrme forces do not alter the conclusion.

For boson system, we consider the IBM-2, because it is closer to a microscopic picture than the simpler version of IBM. The IBM-2 is comprised of proton $L = 0^+ (s_x)$ and $2^+ (d_\pi)$ bosons, and of neutron $L = 0^+ (s_\nu)$ and $2^+ (d_\nu)$ bosons \cite{8}. We take the standard IBM-2 Hamiltonian,

$$H_B = c n_d + \kappa Q_x \cdot Q_{\nu}, \quad (1)$$

where $n_d = n_{d_x} + n_{d_\pi}$ with $n_{d_x} (n_{d_\pi})$ being the proton (neutron) d-boson number operator and $Q_\rho = s_\rho^\dagger d_\rho + d_\rho^\dagger s_\rho + \chi_\rho |d_\rho^\dagger d_\rho|^2$. Here $\epsilon$, $\kappa$, and $\chi_{\pi,\nu}$ are parameters, and their values are determined by comparing nucleonic and bosonic PESs following Refs. \cite{8,12}. The boson intrinsic state $|\phi_B\rangle$ is written in general as a coherent state \cite{27,28}

$$|\phi_B\rangle \propto \prod_{\rho = \pi,\nu} (s_\rho^\dagger + \sum_{\mu = \pm 2,\pm 1} a_{\mu\rho} d_\mu^\dagger)^{n_{\rho}} |0\rangle, \quad (2)$$

where $|0\rangle$ and $a_{\mu\rho}$ represent the boson vacuum (inert core) and amplitude, respectively.

We now look into the problem of rotational response. We shall restrict ourselves to nuclei with axially symmetric strong deformation, because this problem is crucial to those nuclei but is not so relevant to the others. An axially symmetric intrinsic state is invariant with respect to the rotation around the symmetry ($z$) axis. This means $a_{\rho\mu} = 0$ for $\mu \neq 0$ in eq. (2) in the case of bosons. Such intrinsic states of nucleons and bosons are supposed to be obtained as the minima of the PESs. Let us now rotate the axially symmetric intrinsic states about the $y$-axis by angle $\beta$. Figure 1 shows the overlap between the intrinsic state $|\phi_X\rangle$ and the rotated one $|\phi_X^{\beta}\rangle = e^{-iL_\beta}|\phi_X\rangle$, where $X$ stands for either fermion ($X = F$) or boson ($X = B$). Here $L_\beta$ denotes the $y$-component of the angular momentum operator. We take $^{146-154}$Sm and $^{230-238}$U as examples. Some of these nuclei are good examples of SU(3) limit of IBM \cite{23}.

Figures (a,c) and (b,d) show the overlaps for nucleons and bosons, respectively. For Sm isotopes, the parameters of $H_B$ are taken from \cite{12}, while the parameters for U isotopes are determined as $\epsilon \approx 0.100$ MeV, $\kappa \approx -0.18$ MeV, and $\chi_{\pi} \approx \chi_\nu \approx -1.0$. These parameters are used throughout this paper.

In each case, the overlap is peaked at $\beta = 0^\circ$ with the value unity, and decreases with $\beta$. The nucleonic overlaps are peaked more sharply, whereas boson ones are damped more slowly. It is clear that as a function of $\beta$, boson rotated intrinsic state changes more slowly than the corresponding nucleon one, due to limited degrees of freedom for bosons.

We point out that the overlap becomes narrower in $\beta$ with the neutron number $N$ for Sm isotopes (see Fig. (a,b)). This is related to the growth of deformation. On the other hand, there is no notable change in the overlap for these U isotopes, because pronounced prolate minimum appears always at $\beta_2 \sim 0.25$ in their PES.

The nucleon-boson difference of the rotational response discussed so far suggests that the rotational spectrum of a nucleonic system may not be fully reproduced by the boson system determined by the mapping method of Ref. \cite{8} using the PESs at rest. In fact, it will be shown later that the moment of inertia of a nucleon system differs from the one calculated by the mapped boson Hamiltonian. We then introduce a term into the boson Hamiltonian, so as to keep the PES-based mapping procedure but incorporate the different rotational responses. This term takes the form of $\hat{L} \cdot \hat{L}$ where $\hat{L}$ denotes the boson angular momentum operator. This term is nothing but the squared magnitude of the angular momentum with the eigenvalue $L (L + 1)$, and changes the moment of inertia of rotational band keeping their wave functions. A phenomenological term of this form was used in the fitting calculation of IBM, particularly in its SU(3) limit \cite{25}, without knowing its origin or physical significance.

We adopt, hereafter, a Hamiltonian, $H_B'$, which includes this term with coupling constant $\alpha$:

$$H_B' = H_B + \alpha \hat{L} \cdot \hat{L}, \quad (3)$$

where $H_B$ is given in Eq. (1). The $\alpha \hat{L} \cdot \hat{L}$ term will be referred to as LL term hereafter. The LL term contributes to the PES in the same way as a change of $d$-boson energy $\Delta \epsilon = 6\alpha$ (see eq. (1)), because the PES at rest (i.e., $\omega = 0$) is formed by the boson intrinsic state $|\phi_B\rangle$ containing no $d_{\pm 1}$ component. Hence, by shifting $\epsilon$ slightly, we obtain the same PES as the one without the LL term, and consequently the other parameters of mapped $H_B$ remain unchanged.

We now turn to the determination of $\alpha$ in Eq. (3). First, we perform the cranking model calculation for the
fermion system to obtain its moment of inertia, denoted by $J_F$, in the usual way \[ J_F = 2 \cdot \sum_{i,j>0} \frac{|\langle i| L_k | j \rangle|^2}{E_i + E_j} (u_i v_j - u_j v_i)^2, \] where energy $E_i$ and v-factor $v_i$ of quasi-particle state $i$ are calculated by the HF+BCS method of Ref. \[31\]. Here, $L_k$ is the nucleon angular momentum operator, and $k$ means the axis of the cranking rotation, being either $x$ or $y$, as $z$-axis. Based on the earlier argument, the $y$-axis is chosen.

Next, the bosonic moment of inertia, denoted as $J_B$, is calculated by the cranking formula of Ref. \[32\] with $\Delta \pm 1$ being mixed, to an infinitesimal order, into the coherent state $|\phi_B \rangle$ in Eq. \[4\]:

\[ J_B = \lim_{\omega \to 0} \frac{1}{\omega} \langle \phi_B | L_k | \phi_B \rangle, \]

where $\omega$ is the cranking frequency, $a_{\Delta \pm 1}$ denotes the amplitude for $\Delta \pm 1$, and $L_k$ stands for the boson angular momentum operator. Note that $a_{\Delta \pm 1} \propto \omega$ at this limit, leading $J_B$ to a finite value. The value of $\alpha$ is determined for individual nucleus so that the corresponding bosonic moment of inertia, $J_B$ in eq. \[5\] becomes equal to $J_F$ in eq. \[2\]. This prescription makes sense, if the nucleus is strongly deformed and the fixed intrinsic state is so stable as to produce individual levels of a rotational band through the angular momentum projection in a good approximation. The resultant excitation energies should follow the rotor formula $E_\omega \propto L(L+1)$ for $L$ being the angular momentum of the level. The present prescription with the LL term should be applied only to certain nuclei which belong to this type. We introduce a criterion to select such nuclei in terms of the ratio $R_{4/2} = E_\omega(4^+_1)/E_\omega(2^+_1)$, and set a minimum value for this. Empirical systematics \[33\] suggests that the evolution towards stronger deformation continues as the number of valence nucleons increases, but this evolution becomes saturated beyond $R_{4/2} \sim 3.2$. Namely, for the nuclei with $R_{4/2} > 3.2$, the deformation is considered to be evolved sufficiently well, and we take $R_{4/2} > 3.2$ as the criterion to apply the LL term. This discrete criterion is also for the sake of simplicity, but the major discussions of this work do not depend on its details.

Figures \[2\] (a) $\sim$ (c) show the moments of inertia for Sm and U isotopes. In these figures, $J_B$ calculated with the LL term (w/ LL), $J_B$ calculated without it (w/o LL), and $J_F$ are compared. Experimental ones determined from the $2^+_1$ levels \[33\] are shown also.

We divide Sm isotopes into two categories according to the criterion defined above. First, the ratio $R_{4/2}$ is calculated without the LL term, leading to $152-158$ Sm with $R_{4/2} > 3.2$ and $146-150$ Sm with $R_{4/2} < 3.2$. For the former category, the LL term should be included, and...
normalizing it with respect to the $E_x(2^+_1)$ without the LL term, for (a) Sm and (b) U isotopes. This lowering is, as indicated by the arrows in Fig. 3, $>30\%$ for $92\sim96$ Sm and $>60\%$ for $^{140\sim144}$U. On the other side, it is almost vanished or quite small for $N=84\sim90$. Thus, it may not affect the IBM description much, even if one keeps the LL term in all nuclei. We do not take it, because the present derivation does not give physical basis for the LL term for nuclei without strong deformation.

Figure 5 shows yrast levels of $^{154}$Sm, $^{156}$Gd, $^{230}$Th and $^{232}$U nuclei as representatives of rotational nuclei. The LL term is included for these nuclei, as they fulfill the criterion. For $^{230}$Th, the parameters of $H_B$ take almost the same values as those for the $^{232}$U nucleus. A nice overall agreement arises between the theoretical and the experimental spectra, and the contribution of the LL term to it is remarkable. Particularly for $^{154}$Sm and $^{230}$Th, the calculated spectra look nearly identical to the experimental ones.

We comment on side-band levels. The deviations of $\beta$-bandhead ($0^+_2$) and $\gamma$-bandhead ($2^+_2$) energies are improved by tens of keV by the LL term. However, these band-head energies are still much higher than experimental ones. Thus, there are still open questions on side-band levels. On the other hand, the relative spacing inside the bands is reduced by hundreds of keV, producing certain improvements.

We mention some studies deriving a collective Hamiltonian from a given EDF where the mean-field PES supplemented with zero point rotational and vibrational corrections are treated as an effective potential. A generalized kinetic energy term emerges in such approaches. In the present work, we compare the results of Skyrme
EDF with the corresponding results of the mapped boson system, at the levels of the PES and the rotational response. The kinetic energies of nucleons are included in both levels, while the rotational kinetic-like boson term appears from the latter.

In summary, we have proposed a novel formulation of the IBM for rotational nuclei. The rotation of strongly deformed multi-nucleon system differs, in its response to the rotational cranking, from its boson image obtained by the mapping method of Ref. 8 where the PES at rest is considered. Significant differences then appear in moment of inertia between nucleon and boson systems. We have shown that this problem is remedied by introducing the LL term into the IBM Hamiltonian. The effect of the LL term makes essential contribution to rotational spectra, solving the longstanding problem of too small moment of inertia microscopically. Experimental data are reproduced quite well, without any phenomenological adjustment. The mapping of Ref. 8 appears quite sufficient for vibrational and γ-unstable nuclei, and the present study makes the IBM description of strongly deformed nuclei sensible theoretically and empirically. Thus, we seem to have come to the stage of having microscopic basis of the IBM in all situation at the lowest order. On the other hand, this achievement is partly due to the successful description of Skyrme mean-field model. The feature discussed in this paper is related to the question as to whether the IBM can be applied to deformed nuclei or not 22. The present work indicates that the rotational response is substantially different between fermions and bosons, but the difference can be incorporated into the IBM in a microscopic way.

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