Derivation of IBM Hamiltonian for deformed nuclei

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Abstract.

A Hamiltonian of the Interacting Boson Model (IBM) is determined microscopically starting from the mean-field calculation. The potential energy surface (PES) by the Skyrme mean-field method is mapped onto the PES of the IBM to yield the interaction strengths of the IBM Hamiltonian, by which levels and wave functions of excited states are calculated with good angular momentum and the particle number. The response of the rotating nucleon system is mapped onto the corresponding boson system in order to determine the coefficient of the rotational kinetic-like \( \hat{L} \cdot \hat{L} \) term microscopically. By the present method, not only the three dynamical symmetries of IBM but also the recently proposed critical-point symmetries of shape-phase transitions are well reproduced. In particular, the experimental rotational band of the SU(3) nucleus in Sm isotopic chain is reproduced quite nicely. We also point out the quantum fluctuation effect on the binding energies, which is included by the diagonalization of the IBM Hamiltonian determined by the comparison to the Skyrme PES. Systematic results for spectra for Os isotopes are also presented.

1. Introduction

The quadrupole collectivity in atomic nucleus exhibits distinct regularities, where the nuclear shape can be spherical, deformed and the situation in between. Like other models and theories [1, 2], the Interacting Boson Model [3] has been successful in reproducing the nuclear collective levels in terms of \( s \) and \( d \) bosons, which are essentially the collective \( S \) and \( D \) pairs of valence nucleons [4], respectively. If the interaction strengths of the IBM Hamiltonian take specific values, namely if the Hamiltonian has the so-called dynamical symmetry, then the shape of quadrupole deformation can be classified into any of spherical vibrator (U(5)), axially symmetric deformation (SU(3)), and \( \gamma \)-unstable deformation (O(6)). However, since most realistic nuclei are in the intermediate situations among the three limits, the spectra and the transition strengths are calculated numerically, where the IBM Hamiltonian has been determined only phenomenologically so as to reproduce the experimental data. On the other side, the IBM itself has a certain microscopic foundation starting from the nucleon degrees of freedom. It has been usually studied by means of the nuclear shell model. An well-known example can be the OAI mapping method proposed by T. Otsuka, A. Arima and F. Iachello [4], which has been, however, limited to nearly-spherical and \( \gamma \)-unstable nuclei. Thereby, for general situations
including strong deformation, the derivation of the IBM Hamiltonian has remained open for many years.

The limitation of this type of approach is probably because of the fact that the shell-model state, which has been truncated by a generalized seniority scheme [5, 6], contains so complicated information on various many-body effects that it becomes unfeasible in practice particularly for deformed nuclei. On the other side, the potential energy surface in the \( \beta-\gamma \) plane by the mean-field methods seems to have a more direct connection to the quadrupole deformation and appears to be suitable as a starting point for constructing a model Hamiltonian for the description of low-lying states. One of the most successful and well-established mean-field models of nuclei is of the Skyrme-type, which have been useful for the description of various intrinsic-state properties of a nucleus: mass, density distributions, surface deformation, etc [2, 9, 10, 11]. While a given Skyrme interaction appears to give a basic and systematic description of matter and bulk properties of almost all nuclei on the nuclear chart, it has not been so easy in general to calculate levels and wave functions of excited states with the precise treatment of the particle number and the angular momentum.

Recently we have proposed a new approach to determine a Hamiltonian of the IBM starting from the mean-field calculation [7,8]. In this paper, we shall apply this method to see how the low-lying states, in particular those for deformed nuclei, and the shape-phase transitions.

2. Formalism

We now turn to the IBM description of the PES. The following discussion is focused on the proton-neutron IBM (or IBM-2) [4] because it is closer to the microscopic picture. We use the following boson Hamiltonian

\[
\hat{H}_{\text{IBM}} = E_0 + \epsilon (\hat{n}_{d\pi} + \hat{n}_{d\nu}) + \kappa \hat{Q}_{\pi}^{x\pi} \cdot \hat{Q}_{\nu}^{y\nu} + \alpha \hat{L} \cdot \hat{L},
\]

where \( E_0, \hat{n}_{d\rho}, \hat{Q}_{\rho} = [s_{\rho}^+ \times \hat{d}_{\rho} + a_{\rho}^+ \times \hat{d}_{\rho}]^{(2)} \) and \( \hat{Q}_{\rho} = \chi_{\rho} \hat{d}_{\rho} \) stand for the constant term which contributes only to the binding energy, \( d\)-boson number operator with coefficient \( \epsilon \) and the quadrupole operator with strength \( \kappa \), respectively. The forth term represents the rotational kinetic term, which we denote as \( \hat{L} \cdot \hat{L} \) term, hereafter, where \( \hat{L} = \hat{L}_{\pi} + \hat{L}_{\nu} \) is the angular momentum operator with \( \hat{L}_{\rho} \) being \( \hat{L}_{\rho} = \sqrt{10}[d_{\rho}^+ \times \hat{d}_{\rho}]_{\mu(1)} \). The IBM PES is given by the expectation value \( \langle \hat{H}_{\text{IBM}} \rangle | \Phi \rangle \end{document}
We determine the values of the four parameters which appear in the boson Hamiltonian, together with the coefficient $C_\beta$ of Eq. (2) so that the PES of IBM reproduces that of the mean-field calculation. Practically, this is done by the wavelet method [16], which is a sort of the Fourier transform but is a more efficient way to extract the characteristic features of a given signal such as those derived from the PES fits, which are taken from Ref. [8], because there is no need to breaking of the rotational invariance, while other components, to a deformation variable $\beta$ ($\gamma$), which correspond to frequency and position, respectively. The wavelet transform of the PES in $\beta$ direction (for fixed $\gamma$) $\tilde{E}(\delta\beta, \beta)$ is formulated as

$$\tilde{E}(\delta\beta, \beta) = \frac{1}{\sqrt{\delta\beta}} \int E(\beta', \gamma) \Psi^* \left( \frac{\beta - \beta'}{\delta\beta} \right) d\beta',$$

where $\Psi^*$ is a complex conjugate of a wavelet function. $E(\beta', \gamma)$ stands for the PES of either the HF or the IBM. Here the wavelet transform $\tilde{E}(\delta\beta, \beta)$ is in general a complex value. For $\gamma$ direction, one has only to replace $\beta$ ($\delta\beta$) with $\gamma$ ($\delta\gamma$) in Eq. (3). The values of the five parameters $\epsilon$, $\kappa$, $\chi_{\pi,\nu}$ and $C_\beta$ are determined by the $\chi$-square fit of the squared Wavelet transform of the IBM PES $|\tilde{E}|^2$ to that of the mean-field calculation. This process is nothing but the mapping of the HF PES onto the corresponding IBM PES. Here the HF PES reflects the effects of the basic features of nucleon system such as nuclear force and Pauli principle. By the mapping of the PES, such important properties of nucleon system is supposed to be simulated in terms of bosonic degrees of freedom. Using the parameters determined in the above-mentioned way, energy spectra and the transition strengths can be obtained with good angular momentum and the particle number, which enables one to make a spectroscopic predictions.

In a standard microscopic approach to collective motions, a kinetic mass term is considered independently of a potential term in order to calculate the excitation levels [2]. On the other hand, we compare the total energy of the HF+BCS with that of the IBM, where the effect of the mass term can be included to a certain extent by the diagonalization of the IBM Hamiltonian. However, this is not the case with strong deformation as illustrated by the following simple picture. If one rotates a nucleus around an axis in the intrinsic frame which is perpendicular to the symmetry axis of the nucleus, then the overlap of the intrinsic wave functions of rotated and non-rotated states can be defined. For strong deformation, such a overlap of the nucleon wave function is supposed to somewhat differ from the corresponding boson wave function. This difference of the intrinsic wave function requires one to introduce the mass term or the $\hat{L} \cdot \hat{L}$ term in the boson Hamiltonian. Here we note that the $\hat{L} \cdot \hat{L}$ term cannot be determined by the comparison of the PES because it does not contribute to the PES. Then we should formulate the response of the rotating nucleon system and map it onto the corresponding boson system in order to determine the coefficient of $\hat{L} \cdot \hat{L}$ term. We actually carry out the cranking calculation and compare the moments of inertia (MOI) in the intrinsic state between mean-field and IBM. The MOI for nucleon system is obtained by using the Inglis-Belyaev formula [17, 18], based on the Skyrme HF+BCS calculation [20, 21]. The MOI for IBM is obtained by the evaluation of the Inglis-Belyaev formula [17, 18], based on the Skyrme HF+BCS calculation [20, 21]. The MOI for IBM is obtained by the evaluation of the Inglis-Belyaev formula [17, 18], based on the Skyrme HF+BCS calculation [20, 21].
where \( L_{xp} = \frac{\partial (L_{xx})}{\partial a_{x1}} \), \( E_{\rho} = \frac{\partial^2 (\hat{H}_{\text{IBM}})}{\partial a_{\rho}^2} \) and \( E_{\pi_1} = \frac{\partial^2 (\hat{H}_{\text{IBM}})}{\partial a_{\pi_1} \partial a_{\pi_1}} \). We determine the strength of the \( \hat{L} \cdot \hat{L} \) term for individual nucleus so that the IBM MOI of Eq. (4) reproduces that of Inglis-Belyaev formula.

3. Numerical results

3.1. Low-lying states of Sm isotopes

Figure 1 shows the evolutions of low-lying states as functions of neutron number, \( N \). In the present calculation, which is indicated by “IBM(SkM*)” in Fig. (1), the yrast levels decrease with \( N \), while the side-band, \( 0^+_2 \) and \( 2^+_2 \) levels are pushed up at \( N=88 \) or 90, consistently with the experiments (Expt.). One obviously sees in the behaviors of the low-lying states the phase transition from spherical to deformed shapes, together with the X(5) critical point [23].

![Figure 1](image1.png)

**Figure 1.** Low-lying spectra for Sm isotopes as functions of the neutron number \( N \).

For higher-lying yrast levels for Sm isotopes of Fig. 2(a), one sees nice agreement between the calculation and the experimental data up to \( 8^+_1 \) state. Fig. 2(b) shows the level scheme for \( N=96 \) nucleus. This is to show how important the contribution of the \( \hat{L} \cdot \hat{L} \) is on the rotational spectra by showing the cases in which the \( \hat{L} \cdot \hat{L} \) is (IBM+LL) and is not (IBM) included.

![Figure 2](image2.png)

**Figure 2.** Same as Fig. 1, but for (a) the yrast spectra with higher angular momenta, where the curves and symbols represent the calculated and the experimental [22] values. (b) Yrast spectra for \( ^{158}\text{Sm} \) nucleus in the cases in which the \( \hat{L} \cdot \hat{L} \) is (IBM+LL) and is not (IBM) included.

3.2. Binding energy systematics

Now, we focus our discussion on the property of the binding energy. The binding energy of the IBM system is nothing but the eigenenergy of the Hamiltonian of Eq. (1), where the value of the constant term \( E_0 \) is determined for individual nucleus so that the energy minimum in the intrinsic state \( \langle \hat{H}_{\text{IBM}} \rangle \) is adjusted to the energy of the mean-field minimum. Figure 3 shows the deviations of the calculated binding energies for Sm isotopes from the experiments as functions of \( N \). The results based on the Skyrme SkM* and SLy4 forces are shown. The dotted curves show the total energy or equivalently the potential minima of mean-field calculations. The solid curves represents the binding energy obtained by the diagonalization of the IBM Hamiltonian which are calibrated with the mean-field PES. Therefore, the difference between the mean-field and IBM corresponds to the quantum mechanical correlation effect which comes from the exact
treatment of the angular momentum and the particle number in the IBM calculation. The correlation energy is most enhanced for nuclei corresponding to nearly-spherical to transitional regions. In addition, the binding energy of the IBM shows linear behavior as a function of $N$ even at the shell closure. This smoothness of the binding energy due to the correlation effect enables one to describe the two-neutron separation energy better than the case otherwise, as seen in the lower panel of Fig. 3.

![Graph showing deviations of binding energies and two-neutron separation energies for Sm isotopes.](image)

Figure 3. (Upper) Deviations of the calculated binding energies for Sm isotopes from experiments [24]. (Lower) Two-neutron separation energies ($S_{2n}$) for Sm isotopes. Experimental data are indicated by open circles.

3.3. Level evolution in Os isotopes

Now we show the application to other mass region. Figure 4 illustrates the level evolution of $^{76}$Os isotopes with $N=86-122$, where curves and symbols represent the present calculation and the experimental data [22], respectively. The Skyrme SkM* force is used. The calculated yrast levels come down as the number of valence neutrons increases, being consistent with the data. In particular, the $2_1^+$ and $4_1^+$ energies for $N=122$ nucleus in the present calculation are in rather good agreement with the recent experiment [25]. One sees similar kinks of side band levels $0_2^+$

![Graph showing level evolution for Os isotopes.](image)

Figure 4. Same as Fig. 1, but for Os isotopes with $N=86-122$. Skyrme SkM* interaction is used.
and $2^+_2$ to Sm isotopes, which reflect the transition from spherical to deformed shapes. These side-band levels remain higher than $4^+_1$ states around the middle of the major shell, characteristic of the deformed structure which is rather soft and weak as compared to Sm isotopes.

4. Conclusions
To summarize, we illustrated a mean-field-based formulation of the IBM, which has been developed recently, and its application to deformed nuclei. The interaction strengths of the IBM Hamiltonian relevant to the quadrupole collectivity are determined by mapping the PES of Skyrme onto the corresponding IBM PES. In addition, the rotational kinetic-like $\hat{L} \cdot \hat{L}$ term is embedded in the IBM Hamiltonian, and the coefficient of the $\hat{L} \cdot \hat{L}$ term is derived microscopically so that the response of the rotating nucleon system is reproduced by the corresponding boson states. Levels and wave functions of excited states are calculated with good angular momentum and the particle number. This allows one to describe the low-lying states of various cases of quadrupole deformation, including the relevant shape-phase transitions, as well as to evaluate the correlation effect in the binding energy.

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