

Microscopic derivation of the quadrupole collective Hamiltonian for shape coexistence/mixing dynamics

This content has been downloaded from IOPscience. Please scroll down to see the full text.

2016 J. Phys. G: Nucl. Part. Phys. 43 024006

(<http://iopscience.iop.org/0954-3899/43/2/024006>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 130.54.110.31

This content was downloaded on 16/01/2016 at 07:31

Please note that [terms and conditions apply](#).

Microscopic derivation of the quadrupole collective Hamiltonian for shape coexistence/mixing dynamics

Kenichi Matsuyanagi^{1,2}, Masayuki Matsuo³,
Takashi Nakatsukasa^{1,4}, Kenichi Yoshida⁵,
Nobuo Hinohara^{4,6} and Koichi Sato¹

¹RIKEN Nishina Center, Wako 351-0198, Japan

²Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto 606-8502, Japan

³Department of Physics, Faculty of Science, Niigata University, Niigata 950-2181, Japan

⁴Center for Computational Sciences, University of Tsukuba, Tsukuba 305-8571, Japan

⁵Graduate School of Science and Technology, Niigata University, Niigata 950-2181, Japan

⁶National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, MI 48824-1321, USA

Received 4 July 2015, revised 20 August 2015

Accepted for publication 3 September 2015

Published 14 January 2016



CrossMark

Abstract

Assuming that the time-evolution of the self-consistent mean field is determined by five pairs of collective coordinate and collective momentum, we microscopically derive the collective Hamiltonian for low-frequency quadrupole modes of excitation. We show that the five-dimensional collective Schrödinger equation is capable of describing large-amplitude quadrupole shape dynamics seen as shape coexistence/mixing phenomena. We focus on basic ideas and recent advances of the approaches based on the time-dependent mean-field theory, but relations to other time-independent approaches are also briefly discussed.

Keywords: collective Hamiltonian, large-amplitude collective motion, shape coexistence, time-dependent self-consistent mean field

(Some figures may appear in colour only in the online journal)

1. Introduction

In this paper, we focus on low-frequency quadrupole motions which play the major role in low-energy excitation spectra. As is well known, various giant resonances appearing in highly

excited states are well described by the random-phase approximation (RPA), which is a small-amplitude approximation of the time-dependent Hartree–Fock (TDHF) theory. In contrast to the giant resonances, low-frequency quadrupole vibrations exhibit characteristic features associated with superfluidity of the finite quantum system (nucleus), that is, pairing correlations and varying shell structure of the self-consistent mean field play essential roles [1–4].

1.1. Quantum shape fluctuation, shape mixing and shape coexistence

The low-frequency quadrupole vibrations can be regarded as soft modes of the quantum phase transition towards equilibrium deformations of the mean field. As is well known, in nuclei situated in the transitional region from spherical to deformed, amplitudes of quantum shape fluctuation about the equilibrium remarkably increase. This is the case also for weakly deformed nuclei where the gain in binding energies due to the symmetry breaking is comparable in magnitude to the vibrational zero-point energies. The transitional region is wide and those nuclei exhibit quite rich excitation spectra. This is a characteristic feature of finite quantum systems and provides an invaluable opportunity to investigate the process of the quantum phase transition through analysis of quantum spectra. To describe such large-amplitude collective motions (LACM), we need to go beyond the small-amplitude approximation (quasiparticle RPA (QRPA)) of the time-dependent Hartree–Fock–Bogoliubov (TDHFB) theory for superfluid systems. It is required to develop a microscopic theory of LACM capable of describing the varying shell structure associated with the time-dependent mean field with superfluidity.

The spherical shell structure gradually changes with the growth of deformation and generates ‘deformed shell structures’ and ‘deformed magic numbers,’ that stabilize certain deformed shapes of the mean field. When a few local minima of the mean field with different shapes appear in the same energy region, LACM tunneling through potential barriers and extending between local minima may take place. These phenomena may be regarded as a kind of macroscopic quantum tunneling. Note that the barriers are not generated by external fields but self-consistently generated as a consequence of quantum dynamics of the many-body system under consideration. Quantum spectra of low-energy excitation that needs such concepts have been observed in almost all regions of the nuclear chart [5]. When different kinds of quantum eigenstates associated with different shapes coexist in the same energy region, we may call them ‘*shape coexistence phenomena*.’ This is the case when shape mixing due to tunneling motion is weak and collective wave functions retain their localizations about different equilibrium shapes. On the other hand, if the shape mixing is strong, large-amplitude shape fluctuations (*delocalization* of the collective wave functions) extending to different local minima may occur.

1.2. Collective rotations restoring broken symmetries

As is well known, the central concept of the BCS theory of superconductivity is spontaneous breaking of the gauge symmetry and emergence of collective modes. The massless modes restoring the broken symmetry are called Anderson–Nambu–Goldstone (ANG) modes [6–8]. As emphasized by Bohr and Mottelson, nuclear rotation can be regarded as an ANG mode restoring the broken rotational symmetry in real space [1, 9].

In finite quantum systems such as nuclei, the rotational ANG modes may couple rather strongly with quantum shape-fluctuation modes. For instance, even when the self-consistent mean field acquires a deep local minimum at a finite value of β , the nucleus may exhibit a large-amplitude shape fluctuation in the γ degree of freedom, if the deformation potential is

flat in this direction. Here, as usual, β and γ represent the magnitudes of axially symmetric and asymmetric quadrupole deformations, respectively. Such a situation is widely observed in experiments and called γ -soft. Although the quantum-mechanical collective rotation is forbidden about the symmetry axis, the rotational degrees of freedoms about three principal axes are all activated once the axial symmetry is dynamically broken due to the quantum shape fluctuation. Rotational spectra in such γ -soft nuclei do not exhibit a simple $I(I + 1)$ pattern. Such an interplay of the shape-fluctuation and rotational modes may be regarded as a characteristic feature of finite quantum systems and provides an invaluable opportunity to investigate the process of the quantum phase transition through analysis of quantum spectra.

Thus, we need to treat the two kinds of collective variables, i.e., those associated with the symmetry-restoring ANG modes and those for quantum shape fluctuations, in a unified manner to describe low-energy excitation spectra of nuclei.

1.3. Five-dimensional (5D) quadrupole collective Hamiltonian

Vibrational and rotational motions of the nucleus can be described as time-evolution of a self-consistent mean field. This is the basic idea underlying the unified model of Bohr and Mottelson [10, 11]. In this approach, the 5D collective Hamiltonian describing the quadrupole vibrational and rotational motions is given by [1, 12]

$$H_{\text{coll}} = T_{\text{vib}} + T_{\text{rot}} + V(\beta, \gamma), \quad (1)$$

$$T_{\text{vib}} = \frac{1}{2}D_{\beta\beta}(\beta, \gamma)\dot{\beta}^2 + D_{\beta\gamma}(\beta, \gamma)\dot{\beta}\dot{\gamma} + \frac{1}{2}D_{\gamma\gamma}(\beta, \gamma)\dot{\gamma}^2, \quad (2)$$

$$T_{\text{rot}} = \sum_k \frac{I_k^2}{2\mathcal{J}_k(\beta, \gamma)}. \quad (3)$$

Here, β and γ are treated as dynamical variables, and $\dot{\beta}$ and $\dot{\gamma}$ represent their time-derivatives. They are related to expectation values of the quadrupole operators (with respect to the time-dependent mean-field states) and their variations in time. The quantities ($D_{\beta\beta}$, $D_{\beta\gamma}$, and $D_{\gamma\gamma}$) appearing in the kinetic energies of vibrational motion, T_{vib} , represent inertial masses of the vibrational motion. They are functions of β and γ . The quantities I_k and $\mathcal{J}_k(\beta, \gamma)$ in the rotational energy T_{rot} represent the three components of the angular momentum and the corresponding moments of inertia, respectively. Note that they are defined with respect to the principal axes of the body-fixed (intrinsic) frame that is attached to the instantaneous shape of the time-dependent mean-field.

In the case that the potential energy $V(\beta, \gamma)$ has a deep minimum at a finite value of β and $\gamma = 0^\circ$ (or $\gamma = 60^\circ$), a regular rotational spectrum with the $I(I + 1)$ pattern may appear. In addition to the ground band, we can expect the β and γ bands to appear, where vibrational quanta with respect to the β and γ degrees of freedom are excited. Detailed investigations on the γ -vibrational bands over many nuclei have revealed, however, that they usually exhibit significant anharmonicities (non-linearities) [13]. Also for the β -vibrational bands, it has been known [14–16] that they couple, sometimes very strongly, with pairing-vibrational modes (associated with fluctuations of the pairing gap). Recent experimental data indicate the need for a radical review of their characters [5].

1.4. Collective quantization of time-dependent mean fields

States vectors of time-dependent mean field are kinds of generalized coherent states, and we can rigorously formulate the TDHFB as a theory of classical Hamiltonian dynamical system

of large dimension [17–20]. Because time-evolution of the mean field is determined by the classical Hamilton equations, we cannot describe, within the framework of the TDHFB, quantum spectra of low-lying states and macroscopic quantum tunneling phenomena such as spontaneous fissions and subbarrier fusions. To describe these genuine quantum phenomena, we need to introduce a few collective variables determining the time-evolution of the mean field and quantize them. We refer this procedure ‘*collective quantization*.’

For small-amplitude vibrations about an HFB equilibrium, it is well known that we can introduce collective variables in a microscopic way by solving the QRPA equations. Single-particle spectra for a mean-field of a finite quantum system have rich shell structures, and thereby a variety of collective vibrational modes emerge. Even within the isoscalar quadrupole vibrations, two collective modes appear exhibiting quite different characteristics; the low- (usually first excited 2^+) and high-frequency (giant resonance) modes. One of the merits of the QRPA is that we can determine the microscopic structures of the collective coordinates and momenta starting from a huge number of microscopic (particle–hole, particle–particle, and hole–hole) degrees of freedom. We can thus learn how collective vibrations are generated as coherent superpositions of many two-quasiparticle excitations. Examining the microscopic structure of the low-frequency quadrupole vibrations, we see that the weights of two-quasiparticle excitations near the Fermi surface are much larger than those in the mass quadrupole operators (see, e.g., [21]). This clearly indicates the importance of describing collective modes in a microscopic way. Another merit of the QRPA is that it yields the ANG modes and their collective masses (inertial functions). In this way, we can restore the symmetries broken by the mean-field approximation [8, 22, 23].

It has been one of the longstanding fundamental subjects in nuclear structure physics to construct a microscopic theory of LACM by extending the QRPA concepts to non-equilibrium states [24–26]. Below we shall briefly review various ideas proposed up to now for this aim.

2. Basic ideas of large-amplitude collective motion

During the attempts to construct a microscopic theory of LACM since the latter half of the 1970s, significant progress has been achieved in the fundamental concepts of collective motion. Especially important is the recognition that microscopic derivation of the collective Hamiltonian is equivalent to extraction of a collective submanifold embedded in the TDHFB phase space, which is approximately decoupled from other non-collective degrees of freedom. From this point of view we can say that collective variables are nothing but local canonical variables which can be flexibly chosen on this submanifold. Below we review recent developments achieved on the basis of such concepts.

2.1. Extraction of collective submanifold

Attempts to formulate a LACM theory without assuming adiabaticity of large-amplitude collective motion were initiated by Rowe and Bassermann [27] and Marumori [28], and led to the formulation of the self-consistent collective coordinate (SCC) method [29]. In these approaches, collective coordinates and collective momenta are treated on the same footing. In the SCC method, basic equations determining the collective submanifold are derived by requiring maximal decoupling of the collective motion of interest and other non-collective degrees of freedom. The collective submanifold is a geometrical object that is invariant with respect to the choice of the coordinate system whereas the collective coordinates depend on it. The idea of coordinate-independent theory of collective motion was developed also by Rowe

[30] and Yamamura and Kuriyama [19]. This idea gave a deep impact on the fundamental question ‘*what are the collective variables.*’ The SCC method was first formulated for TDHF, but later extended to TDHFB for describing nuclei with superfluidity [31].

In the SCC method, under the assumption that time evolution is governed by a few collective coordinates $q = (q_1, q_2, \dots, q_f)$ and collective momenta $p = (p_1, p_2, \dots, p_f)$, the TDHFB states vectors are written as

$$|\phi(t)\rangle = |\phi(q, p)\rangle = e^{i\hat{G}(q,p)} |\phi_0\rangle, \quad (4)$$

or equivalently,

$$|\phi(t)\rangle = |\phi(\eta, \eta^*)\rangle = e^{i\hat{G}(\eta, \eta^*)} |\phi_0\rangle, \quad (5)$$

where $|\phi_0\rangle$ denotes the HFB ground state and $\eta = (\eta_1, \eta_2, \dots, \eta_f)$ with

$$\eta_i = \frac{1}{\sqrt{2}}(q_i + ip_i), \quad \eta_i^* = \frac{1}{\sqrt{2}}(q_i - ip_i). \quad (6)$$

The TDHFB states $|\phi(t)\rangle$ are required to fulfill the canonical variable conditions

$$\langle \phi(\eta, \eta^*) | \frac{\partial}{\partial \eta_i} | \phi(\eta, \eta^*) \rangle = \frac{1}{2} \eta_i^*, \quad (7)$$

$$\langle \phi(\eta, \eta^*) | \frac{\partial}{\partial \eta_i^*} | \phi(\eta, \eta^*) \rangle = -\frac{1}{2} \eta_i, \quad (8)$$

which guarantee that (q, p) are canonical conjugate pairs. The one-body operator $\hat{G}(\eta, \eta^*)$ is determined by the time-dependent variational principle

$$\delta \langle \phi(\eta, \eta^*) | i \frac{\partial}{\partial t} - H | \phi(\eta, \eta^*) \rangle = 0 \quad (9)$$

with

$$\frac{\partial}{\partial t} = \sum_i \left(\dot{\eta}_i \frac{\partial}{\partial \eta_i} + \dot{\eta}_i^* \frac{\partial}{\partial \eta_i^*} \right), \quad (10)$$

and the canonical variable conditions.

Making a power-series expansion of \hat{G} with respect to (η, η^*) ,

$$\hat{G}(\eta, \eta^*) = \sum_i \left(\hat{G}_i^{(10)} \eta_i^* + \hat{G}_i^{(01)} \eta_i \right) + \sum_{ij} \left(\hat{G}_{ij}^{(20)} \eta_i^* \eta_j^* + \hat{G}_{ij}^{(11)} \eta_i^* \eta_i + \hat{G}_{ij}^{(02)} \eta_i \eta_j \right) + \dots \quad (11)$$

and requiring that the time-dependent variational principle holds for every power of (η, η^*) , we can successively determine the one-body operators $\hat{G}^{(m,n)}$ with $m+n=1, 2, 3, \dots$. This method of solution is called the (η, η^*) expansion method. The collective Hamiltonian is defined by the expectation value of the microscopic Hamiltonian with respect to $|\phi(\eta, \eta^*)\rangle$. Because (η, η^*) are canonical variables, they are replaced by boson operators after canonical quantization. The lowest linear order corresponds to the QRPA. Accordingly, the collective variables (η_i, η_i^*) correspond to specific QRPA modes in the small-amplitude limit. It is important to note, however, that the microscopic structure of \hat{G} changes as a function of (η_i, η_i^*) due to the mode-mode coupling effects among different QRPA modes in the higher order. In this sense, the SCC method may be regarded as a dynamical extension of the boson expansion method [32]. Thus, the SCC is a powerful method of treating anharmonic effects to the QRPA vibrations originating from mode–mode couplings, as shown in its application to the two-phonon states of anharmonic γ vibration [13, 33]. The SCC method was also used for

derivation of the 5D quadrupole collective Hamiltonian and analysis of the quantum phase transition from spherical to deformed shapes [34], and for constructing diabatic representation in the rotating shell model [35].

2.2. Solution with adiabatic expansion

The (η, η^*) expansion about an HFB equilibrium point is not suitable for treating situations such as shape coexistence, where a few local minima energetically compete in the HFB potential energy surface. For describing adiabatic LACM extending over different HFB local minima, a new method has been proposed [36]. In this method, the basic equations of the SCC method are solved by an expansion with respect to the collective momenta. It is called ‘adiabatic SCC (ASCC) method.’ Similar methods have been developed also by Klein *et al* [37], and Almehed and Walet [38].

Let us assume that the TDHFB state vector can be written as

$$|\phi(q, p)\rangle = e^{i\sum_i p_i \hat{Q}^i(q)} |\phi(q)\rangle. \quad (12)$$

Here, $\hat{Q}^i(q)$ are one-body operators, called infinitesimal generators, and $|\phi(q)\rangle$ is an intrinsic state at the collective coordinate q , called a moving frame HFB state.

We determine the microscopic structures of $\hat{Q}^i(q)$ and $|\phi(q)\rangle$ by the time-dependent variational principle

$$\delta \langle \phi(q, p) | i \frac{\partial}{\partial t} - \hat{H} | \phi(q, p) \rangle = 0. \quad (13)$$

Making power-series expansions with respect to the collective momenta p and retaining terms up to the second order in p , we obtain

moving-frame HFB equation

$$\delta \langle \phi(q) | \hat{H}_M(q) | \phi(q) \rangle = 0, \quad (14)$$

moving-frame QRPA equations (local harmonic equations)

$$\delta \langle \phi(q) | \left[\hat{H}_M(q), \hat{Q}^i(q) \right] - \frac{1}{i} \sum_k B^{ik}(q) \hat{P}_k(q) + \frac{1}{2} \left[\sum_k \frac{\partial V}{\partial q^k} \hat{Q}^k(q), \hat{Q}^i(q) \right] | \phi(q) \rangle = 0, \quad (15)$$

$$\begin{aligned} & \delta \langle \phi(q) | \left[\hat{H}_M(q), \frac{1}{i} \hat{P}_i(q) \right] - \sum_j C_{ij}(q) \hat{Q}^j(q) \\ & - \frac{1}{2} \left[\left[\hat{H}_M(q), \sum_k \frac{\partial V}{\partial q^k} \hat{Q}^k(q) \right], \sum_j B_{ij}(q) \hat{Q}^j(q) \right] | \phi(q) \rangle = 0, \end{aligned} \quad (16)$$

where $\hat{H}_M(q)$ represents the Hamiltonian in the frame attached to the moving mean field,

$$\hat{H}_M(q) = \hat{H} - \sum_i \frac{\partial V}{\partial q^i} \hat{Q}^i(q), \quad (17)$$

and is called ‘moving-frame Hamiltonian.’ The displacement operators $\hat{P}_i(q)$ and $C_{ij}(q)$ are defined by

$$\hat{P}_i(q) | \phi(q) \rangle = i \frac{\partial}{\partial q^i} | \phi(q) \rangle \quad (18)$$

and

$$C_{ij}(q) = \frac{\partial^2 V}{\partial q^i \partial q^j} - \sum_k \Gamma_{ij}^k \frac{\partial V}{\partial q^k}, \quad (19)$$

respectively, with

$$\Gamma_{ij}^k(q) = \frac{1}{2} \sum_l B^{kl} \left(\frac{\partial B_{li}}{\partial q^j} + \frac{\partial B_{lj}}{\partial q^i} - \frac{\partial B_{ij}}{\partial q^l} \right). \quad (20)$$

The double-commutator term in equation (16) arises from the q -derivative of the infinitesimal generators $\hat{Q}^i(q)$ and represents the curvatures of the collective submanifold.

Solving these equations self-consistently, we can determine the microscopic expressions of the infinitesimal generators $\hat{Q}^i(q)$ and $\hat{P}_i(q)$ in bilinear forms of the quasiparticle creation and annihilation operators defined locally with respect to $|\phi(q)\rangle$. The collective Hamiltonian is given by

$$\begin{aligned} \mathcal{H}(q, p) &= \langle \phi(q, p) | \hat{H} | \phi(q, p) \rangle \\ &= V(q) + \frac{1}{2} \sum_{ij} B^{ij}(q) p_i p_j \end{aligned} \quad (21)$$

with

$$V(q) = \mathcal{H}(q, p)|_{p=0}, \quad B^{ij}(q) = \frac{\partial^2 \mathcal{H}}{\partial p_i \partial p_j} |_{p=0}, \quad (22)$$

where $V(q)$ and $B^{ij}(q)$ represent the collective potential and the reciprocals of collective inertial mass, respectively. They are functions of the collective coordinate q . Note that equations (14)–(16) reduce to the HFB and QRPA equations at equilibrium points, where $\partial V / \partial q^i = 0$; namely, they are natural extensions of the HFB-QRPA equations to non-equilibrium states.

Let us note the following points.

- *Difference from the constrained HFB equations.* The moving-frame HFB equation (14) resembles the constrained HFB equation, but the infinitesimal generators $\hat{Q}^i(q)$ are here self-consistently determined together with $\hat{P}_i(q)$ as solutions of the moving-frame QRPA equations (15) and (16) at every point of the collective coordinate q . Thus, contrary to constrained operators in the constrained HFB theory, their microscopic structures change as functions of q . In other words, the optimal ‘constraining’ operators are locally determined at every point of q . The collective submanifold embedded in the TDHFB phase space is extracted in this way. The canonical quantization of the collective Hamiltonian described by a few collective variables (q, p) is similar to the quantization of constrained system [30], but the ‘constraints’ are here generated by the dynamics of the quantum many-body system under consideration.
- *Meaning of the term ‘adiabatic’.* It is used here in the meaning that we can solve the time-dependent variational equation (13) in a good approximation by taking into account up to the second order in an expansion with respect to the collective momenta p . It is important to note that the effects of finite frequency of the LACM are taken into account through the moving-frame QRPA equations. No assumption is made like that the kinetic energy of LACM is much smaller than the lowest two-quasiparticle excitation energy at every point of q .
- *Physics of collective inertial mass.* The collective inertial mass represents the inertia of the many-body system against an infinitesimal change of the collective coordinate q

during the time evolution of the mean field. It is a local quantity and varies as a function of q . As the single-particle-energy spectrum in the mean field changes as a function of q , level crossing at the Fermi energy successively occurs during the LACM. In the presence of the pairing correlation, the many-body system can easily rearrange the lowest-energy configurations at every value of q , i.e., the system can easily change q . The easiness/hardness of the configuration rearrangements at the level crossings determines the adiabaticity/diabaticity of the system. Since the inertia represents a property of the system trying to keep a definite configuration, we expect that the stronger the pairing correlation becomes, the smaller the collective inertial mass becomes [39]. It remains as an interesting subject to investigate how the self-consistent determination of the optimal directions of collective motion and the finite frequency $\omega(q)$ of the moving-frame QRPA modes affect the level-crossing dynamics of the superfluid nuclear systems.

2.3. Consideration of gauge invariance

In the QRPA, the ANG modes such as the number-fluctuation (pairing rotational) modes are decoupled from other normal modes and thereby the QRPA restores the gauge invariance (number conservation) broken in the HFB mean field [8]. It is desirable to keep such a merits of the QRPA beyond the small-amplitude approximation. Otherwise, spurious number-fluctuation modes would unexpectedly mix in the LACM of interest. We can take into account the gauge invariance in the following way [40]. Introducing the number-fluctuation variables $n^{(\tau)}$ and the gauge angles $\varphi^{(\tau)}$ conjugate to them, we write the TDHFB state vector (12) in a more general form:

$$|\phi(q, p, \varphi, n)\rangle = e^{-i\sum_{\tau} \varphi^{(\tau)} \tilde{N}^{(\tau)}} |\phi(q, p, n)\rangle \quad (23)$$

with

$$|\phi(q, p, n)\rangle = e^{i\hat{G}(q,p,n)} |\phi(q)\rangle \quad (24)$$

and

$$\hat{G}(q, p, n) = \sum_i p_i \hat{Q}^i(q) + \sum_{\tau=n,p} n^{(\tau)} \hat{\Theta}^{(\tau)}(q). \quad (25)$$

Here $\tilde{N}^{(\tau)} \equiv \hat{N}^{(\tau)} - N_0^{(\tau)}$ are the number-fluctuation operators measured from $N_0^{(\tau)} \equiv \langle \phi(q) | \hat{N}^{(\tau)} | \phi(q) \rangle$, with the suffix τ distinguishing protons and neutrons, and $\hat{\Theta}^{(\tau)}(q)$ infinitesimal generators for the pairing-rotation degrees of freedom. The state vector $|\phi(q, p, n)\rangle$ may be regarded as an intrinsic state to the pairing rotation. Using $|\phi(q, p, \varphi, n)\rangle$ in place of $|\phi(q, p)\rangle$ in equation (13) and expanding it in $n^{(\tau)}$ as well as p up to the second order, we can determine $\hat{\Theta}^{(\tau)}(q)$ simultaneously with $\hat{Q}^i(q)$ and $\hat{P}^i(q)$ such that the moving-frame HFB + QRPA equations become invariant against the rotation of the gauge angle $\varphi^{(\tau)}$. The gauge invariance of the resulting equations implies that we need to fix a gauge in numerical applications. A convenient procedure of the gauge fixing is discussed in [40].

3. Microscopic derivation of the 5D quadrupole collective Hamiltonian

For collective submanifolds of two dimensions (2D) or more, large-scale numerical computation is needed to find fully self-consistent solutions of the ASCC equations. Then, a practical approximation scheme, called local QRPA (LQRPA) method, has been developed [41–43]. This scheme may be regarded as a first step of iterative solution of equations (14)–

(16). With use of it, we can easily derive the 5D collective Hamiltonian. We first derive the 2D collective Hamiltonian for vibrational motions corresponding to the (β, γ) deformations, and then consider the three-dimensional (3D) rotational motions.

First, we solve the constrained HFB equation

$$\delta \langle \phi(\beta, \gamma) | \hat{H}_{\text{CHFB}}(\beta, \gamma) | \phi(\beta, \gamma) \rangle = 0 \quad (26)$$

with

$$\hat{H}_{\text{CHFB}}(\beta, \gamma) = \hat{H} - \sum_{\tau} \lambda^{(\tau)}(\beta, \gamma) \tilde{N}^{(\tau)} - \sum_{m=0,2} \mu_m(\beta, \gamma) \hat{D}_{2m}^{(+)},$$

where $\lambda^{(\tau)}(\beta, \gamma)$, $\mu_m(\beta, \gamma)$ and $\hat{D}_{2m}^{(+)}$ are the chemical potentials, the Lagrange multipliers, and the quadrupole operators, respectively. The quadrupole deformation parameters (β, γ) are defined by

$$\beta \cos \gamma = \eta D_{20}^{(+)} = \eta \langle \phi(\beta, \gamma) | \hat{D}_{20}^{(+)} | \phi(\beta, \gamma) \rangle, \quad (27)$$

$$\frac{1}{\sqrt{2}} \beta \sin \gamma = \eta D_{22}^{(+)} = \eta \langle \phi(\beta, \gamma) | \hat{D}_{22}^{(+)} | \phi(\beta, \gamma) \rangle, \quad (28)$$

where η is a scaling factor [1, 44].

Next, we solve

$$\delta \langle \phi(\beta, \gamma) | \left[\hat{H}_{\text{CHFB}}(\beta, \gamma), \hat{Q}^i(\beta, \gamma) \right] - \frac{1}{i} \hat{P}_i(\beta, \gamma) | \phi(\beta, \gamma) \rangle = 0, \quad (i = 1, 2) \quad (29)$$

$$\delta \langle \phi(\beta, \gamma) | \left[\hat{H}_{\text{CHFB}}(\beta, \gamma), \frac{1}{i} \hat{P}_i(\beta, \gamma) \right] - C_i(\beta, \gamma) \hat{Q}^i(\beta, \gamma) | \phi(\beta, \gamma) \rangle = 0. \quad (i = 1, 2) \quad (30)$$

These are the moving-frame QRPA equations without the curvature terms and called local QRPA (LQRPA) equations. Making a similarity transformation such that the collective masses corresponding to the collective coordinates (q_1, q_2) become unity, we can write the kinetic energy of vibrational motions as

$$T_{\text{vib}} = \frac{1}{2} \sum_{i=1,2} (p_i)^2 = \frac{1}{2} \sum_{i=1,2} (\dot{q}^i)^2 \quad (31)$$

without loss of generality. Changes of the quadrupole deformation due to variations with respect to (q_1, q_2) are given by

$$dD_{2m}^{(+)} = \sum_{i=1,2} \frac{\partial D_{2m}^{(+)}}{\partial q^i} dq^i. \quad (m = 0, 2) \quad (32)$$

Thus, the kinetic energy of vibrational motions is given in terms of time derivatives of the quadrupole deformation,

$$T_{\text{vib}} = \frac{1}{2} M_{00} \left[\dot{D}_{20}^{(+)} \right]^2 + M_{02} \dot{D}_{20}^{(+)} \dot{D}_{22}^{(+)} + \frac{1}{2} M_{22} \left[\dot{D}_{22}^{(+)} \right]^2, \quad (33)$$

where

$$M_{mm'}(\beta, \gamma) = \sum_{i=1,2} \frac{\partial q^i}{\partial D_{2m}^{(+)}} \frac{\partial q^i}{\partial D_{2m'}^{(+)}}. \quad (34)$$

It is straightforward to rewrite the above expression using the time derivatives of (β, γ) . Subsequently we solve the LQRPA equations for 3D rotational motions at every point on the (β, γ) plane to obtain the inertial functions $D_k(\beta, \gamma)$ and the moments of inertia $\mathcal{J}_k(\beta, \gamma) = 4\beta^2 D_k(\beta, \gamma) \sin^2(\gamma - 2\pi k/3)$ determining the rotational energy T_{rot} . This step is the same as in Thouless and Valatin [45], except that the procedure is applied for non-equilibrium points of (β, γ) as well as the equilibrium points in the potential energy surface $V(\beta, \gamma)$.

After quantizing in curvilinear coordinates (so-called Pauli prescription) [46], we obtain the quantized 5D quadrupole collective Hamiltonian,

$$\hat{H}_{\text{coll}} = \hat{T}_{\text{vib}} + \hat{T}_{\text{rot}} + V(\beta, \gamma), \quad (35)$$

whose vibrational kinetic-energy term takes the following form:

$$\begin{aligned} \hat{T}_{\text{vib}} = & \frac{-\hbar^2}{2\sqrt{WR}} \left\{ \frac{1}{\beta^3} \left[\frac{\partial}{\partial \beta} \left(\beta^3 \sqrt{\frac{R}{W}} D_{\gamma\gamma} \frac{\partial}{\partial \beta} \right) - \frac{\partial}{\partial \beta} \left(\beta^3 \sqrt{\frac{R}{W}} D_{\beta\gamma} \frac{\partial}{\partial \gamma} \right) \right] \right. \\ & \left. + \frac{1}{\sin 3\gamma} \left[-\frac{\partial}{\partial \gamma} \left(\sqrt{\frac{R}{W}} \sin 3\gamma D_{\beta\gamma} \frac{\partial}{\partial \beta} \right) + \frac{\partial}{\partial \gamma} \left(\sqrt{\frac{R}{W}} \sin 3\gamma D_{\beta\beta} \frac{\partial}{\partial \gamma} \right) \right] \right\}, \end{aligned} \quad (36)$$

$$(37)$$

where

$$W = D_{\beta\beta}(\beta, \gamma) D_{\gamma\gamma}(\beta, \gamma) - D_{\beta\gamma}^2(\beta, \gamma), \quad (38)$$

$$R = D_1(\beta, \gamma) D_2(\beta, \gamma) D_3(\beta, \gamma). \quad (39)$$

If the inertial functions ($D_{\beta\beta}$, $D_{\gamma\gamma}$, D_1 , D_2 , D_3) are replaced by a common constant D and $D_{\beta\gamma}$ by 0, the above expression is reduced to

$$\hat{T}_{\text{vib}} = -\frac{\hbar^2}{2D} \left(\frac{1}{\beta^4} \frac{\partial}{\partial \beta} \beta^4 \frac{\partial}{\partial \beta} + \frac{1}{\beta^2 \sin 3\gamma} \frac{\partial}{\partial \gamma} \sin 3\gamma \frac{\partial}{\partial \gamma} \right). \quad (40)$$

Such a drastic approximation may be valid only for small-amplitude vibrations about a spherical HFB equilibrium.

Writing the collective wave functions as

$$\Psi_{\alpha IM}(\beta, \gamma, \Omega) = \sum_{K=\text{even}} \Phi_{\alpha IK}(\beta, \gamma) \langle \Omega | IMK \rangle, \quad (41)$$

$$\langle \Omega | IMK \rangle = \sqrt{\frac{2I+1}{16\pi^2(1+\delta_{K0})}} \left[\mathcal{D}_{MK}^I(\Omega) + (-)^I \mathcal{D}_{M-K}^I(\Omega) \right] \quad (42)$$

and solving the eigenvalue equation for vibrational wave functions

$$\left[\hat{T}_{\text{vib}} + V(\beta, \gamma) \right] \Phi_{\alpha IK}(\beta, \gamma) + \sum_{K'=\text{even}} \langle IMK | \hat{T}_{\text{rot}} | IMK' \rangle \Phi_{\alpha IK'}(\beta, \gamma) = E_{\alpha I} \Phi_{\alpha IK}(\beta, \gamma), \quad (43)$$

we obtain quantum spectra of quadrupole collective motion. The symmetries and boundary conditions of the vibrational wave functions are discussed in [47].

4. Illustrative examples

We here present some applications of the LQRPA method for deriving the 5D collective Hamiltonian. In the numerical examples below, the pairing-plus-quadrupole (P + Q) model Hamiltonian [48] (including the quadrupole-pairing interaction) is employed in solving the CHFB + LQRPA equations. The single-particle energies and the P + Q interaction strengths are determined such that the results of the Skyrme-HFB calculation for the ground states are best reproduced within the P + Q model (see [42, 49] for details). The LQRPA method is quite general and it can be used in conjunction with various Skyrme interactions or modern density functionals. A large-scale calculation is required, however, and such an application of the LQRPA method with realistic interactions/functionals is a challenging future subject. A step toward this goal has recently been carried out for axially symmetric cases [50]. More examples can be found in [41, 51] for $^{68-72}\text{Se}$, [42] for $^{72,74,76}\text{Kr}$, [52] for the ^{26}Mg region, [49] for $^{30-34}\text{Mg}$, [50] for $^{58-68}\text{Cr}$, [43] for $^{58-66}\text{Cr}$, and [53] for $^{128-132}\text{Xe}$ and $^{130-134}\text{Ba}$.

4.1. Oblate–prolate shape coexistence and fluctuations in ^{72}Kr

The collective potential $V(\beta, \gamma)$ depicted in figure 1 exhibits two local minima. The oblate minimum is lower than the prolate minimum. This is expected from the deformed shell structure which gives rise to an oblate magic number at $Z = N = 36$. This figure also shows that the valley runs in the triaxially deformed region and the barrier connecting the oblate and prolate minima is low. Accordingly, one may expect large-amplitude quantum shape fluctuations to occur along the triaxial valley. In fact, the vibrational wave function of the ground 0_1^+ state peaks around the oblate potential minimum, but its tail extends to the prolate region. The vibrational wave function of the excited 0_2^+ state consists of two components: one is a sharp peak on the oblate side and the other is a component spreading around the prolate region somewhat broadly. It is interesting to notice that, as the angular momentum increases, the localization of the vibrational wave functions in the (β, γ) deformation plane develops; namely, the rotational effect plays an important role for the emergence of the shape-coexistence character.

We note that not only the vibrational inertial masses shown in figure 1 but also the rotational inertial functions (D_1 , D_2 , and D_3) and the pairing gaps significantly change as functions of (β, γ) . Due to the time-odd contributions of the moving HFB self-consistent field, the collective inertial masses calculated with the LQRPA method are 20%–50% larger than those evaluated with the Inglis–Belyaev cranking formula. Their ratios also change as functions of (β, γ) [42]. As a consequence, as shown in figure 2, the excitation spectrum calculated with the LQRPA masses is in much better agreement with experimental data than that with the Inglis–Belyaev cranking masses.

4.2. Quantum shape transitions and fluctuations in $^{30,32,34}\text{Mg}$

This is a new region of quantum shape transition currently under live discussions toward understanding the nature of the quadrupole deformation in these neutron-rich isotopes as well as the mechanism of its emergence.

Figure 3 shows the collective potentials $V(\beta, \gamma)$ and the vibrational wave functions squared, $\sum_K |\Phi_{\alpha IK}(\beta, \gamma)|^2$, of the 0_1^+ , 2_1^+ , and 0_2^+ states in $^{30,32,34}\text{Mg}$. It is clearly seen that prolate deformation grows with the neutron number. The deformed magic numbers, $Z = 12$ of protons and $N = 20, 22, 24$ at different values of β of neutrons [56] act cooperatively for the appearance of the prolate minima. Interestingly, the vibrational wave functions of the 2_1^+ state

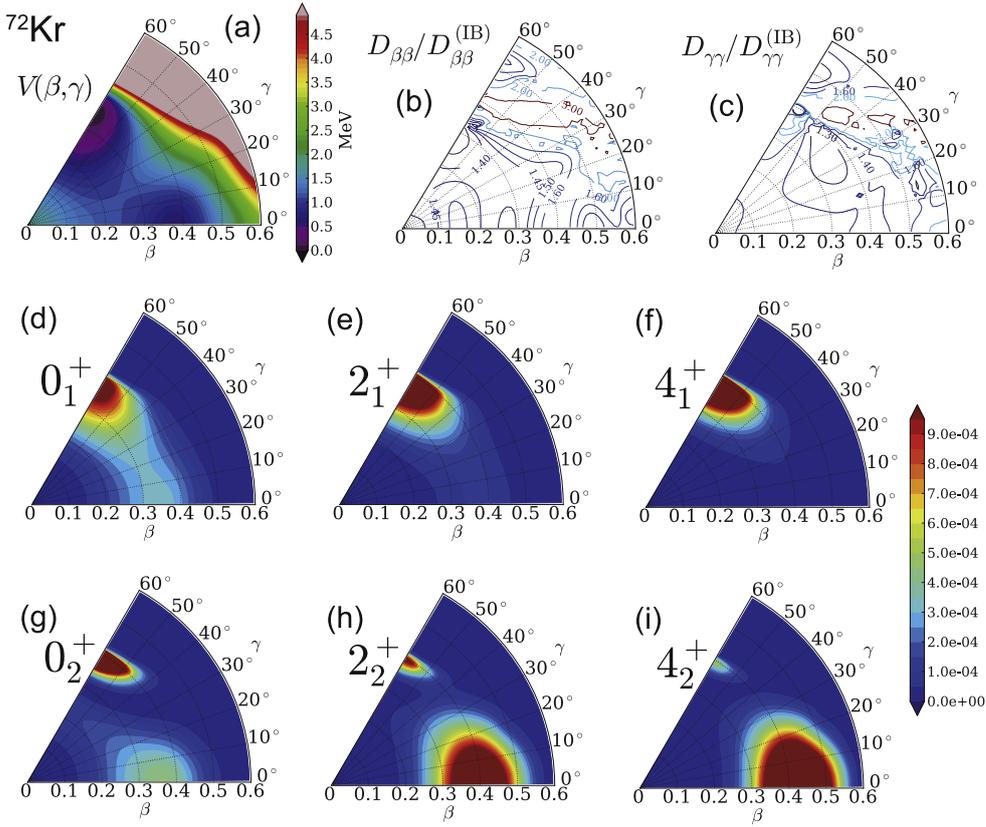


Figure 1. Application of the LQRPA method to the oblate–prolate shape coexistence/fluctuation phenomenon in ^{72}Kr (from [42]). (a) Collective potential $V(\beta, \gamma)$, (b) ratios of the collective inertial masses $D_{\beta\beta}(\beta, \gamma)$ to the Inglis–Belyaev cranking masses. (c) Same as (b) but for $D_{\gamma\gamma}(\beta, \gamma)$. Vibrational wave functions squared, $\sum_K \beta^4 |\Phi_{\alpha IK}(\beta, \gamma)|^2$, for (d) the 0_1^+ state, (e) the 2_1^+ state, (f) the 4_1^+ state, (g) the 0_2^+ state, (h) the 2_2^+ state, and (i) the 4_2^+ state. For the β^4 factor, see the text.

are noticeably different from those of the 0_1^+ state in ^{30}Mg and ^{32}Mg , while they are similar in ^{34}Mg .

In figure 4, we display the probability density of finding a shape with a specific value of β .

$$P(\beta) = \int d\gamma |\Phi_{\alpha I=0, K=0}(\beta, \gamma)|^2 |G(\beta, \gamma)|^{1/2}. \quad (44)$$

Note that the volume element with $|G(\beta, \gamma)| = 4\beta^8 W(\beta, \gamma) R(\beta, \gamma) \sin^2 3\gamma$ is taken into account here. Let us first look at the ground 0_1^+ states. The peak position moves toward a larger value of β in going from ^{30}Mg to ^{34}Mg . The distribution for ^{32}Mg is much broader than those for ^{30}Mg and ^{34}Mg . Next, let us look at the excited 0_2^+ states. In ^{30}Mg , the bump at $\beta \simeq 0.1$ is much smaller than the major bump at $\beta \simeq 0.3$. In this sense, we can regard the 0_2^+ state of ^{30}Mg as a prolately deformed state. In the case of ^{32}Mg , the probability density exhibits a

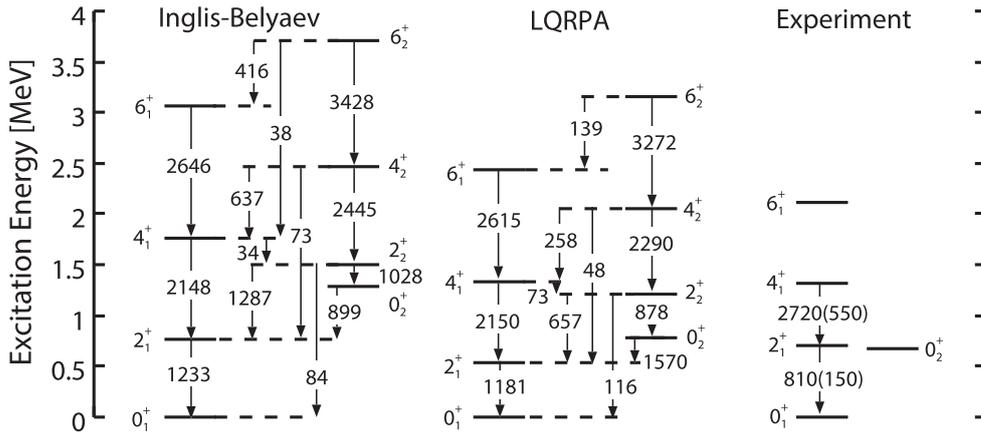


Figure 2. Excitation spectra and $B(E2)$ values calculated for ^{72}Kr by means of the CHB + LQRPA method (denoted by LQRPA) [42] and experimental data [54, 55]. For comparison, the results calculated using the Inglis–Belyaev cranking mass are also shown. Only $B(E2)$ larger than 1 Weisskopf unit are shown in units of $e^2 \text{fm}^4$.

very broad distribution extending from the spherical to deformed regions up to $\beta = 0.5$ with a prominent peak at $\beta \simeq 0.4$ and a node at $\beta \simeq 0.3$.

Thus, the shape coexistence picture that the deformed excited 0_2^+ state coexists with the spherical ground state approximately holds for ^{30}Mg . On the other hand, large-amplitude quadrupole-shape fluctuations dominate in both the ground and the excited 0^+ states in ^{32}Mg , in contrast to the interpretation of deformed ground and spherical excited 0^+ states [57] based on a naive picture of crossing between the spherical and deformed configurations. To test these theoretical predictions, an experimental search for the distorted rotational bands built on the excited 0_2^+ states in ^{30}Mg and ^{32}Mg is strongly desired.

5. Some remarks on other approaches

In section 2, we reviewed the basics of a microscopic theory of LACM focusing on new developments achieved after 2000. In this section, we give short remarks on other approaches to LACM. Typical approaches developed by 1980 are described in detail in the textbook of Ring and Schuck [22], and achievements during 1980–2000 are well summarized in the review by Do Dang, Klein, and Walet [58].

5.1. Constrained HFB + adiabatic perturbation

Historically, the Inglis–Belyaev cranking masses derived from the adiabatic perturbation theory [22] have been widely used in conjunction with phenomenological mean-field models, e.g. for the study of fission dynamics [59]. In recent years, it has become possible to carry out such studies using self-consistent mean fields obtained by solving the constrained HFB equations [60]. The Inglis–Belyaev cranking masses have also been used for low-frequency quadrupole collective dynamics [61–64]. At present, a systematic investigation on low-lying quadrupole spectra is underway using the 5D collective Hamiltonian with Inglis–Belyaev cranking masses and the relativistic (covariant) density functionals [65–71].

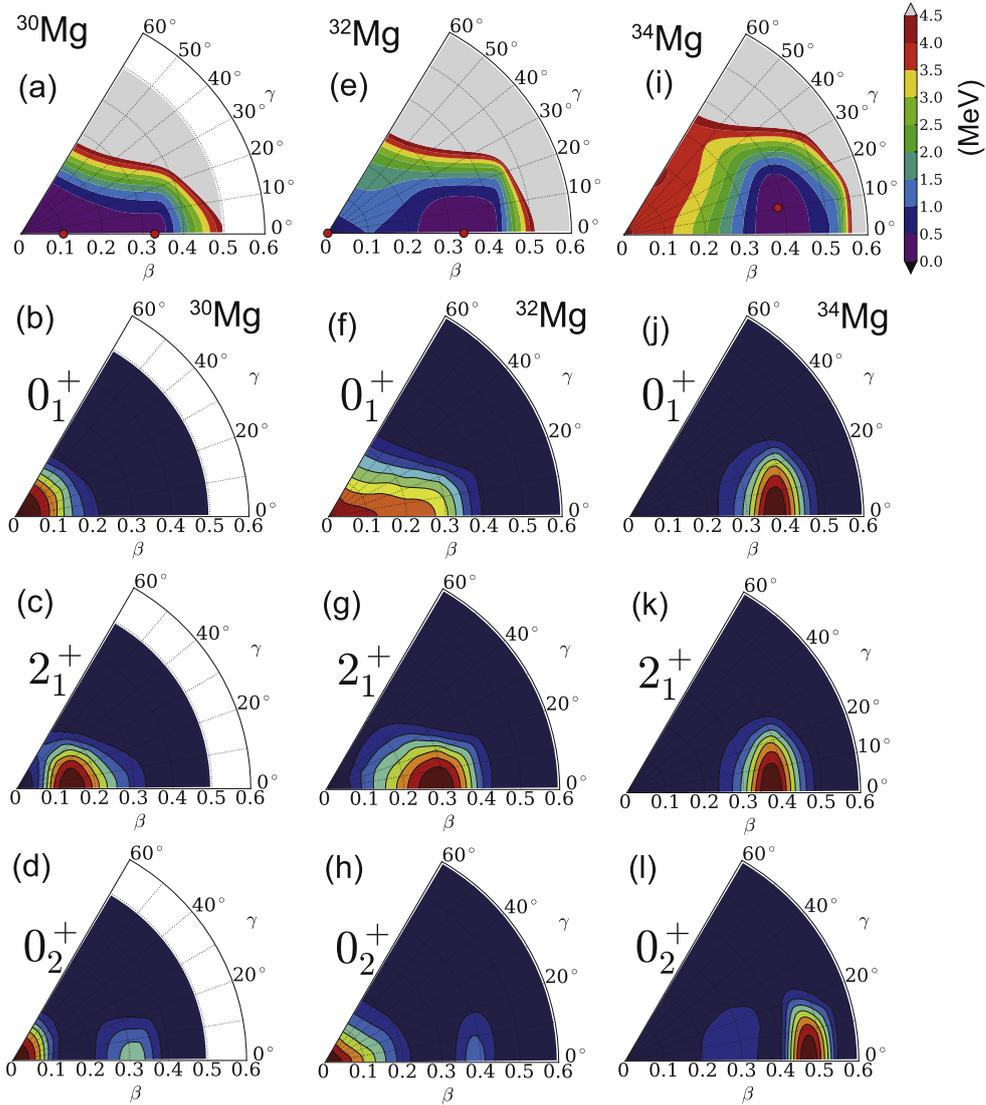


Figure 3. Application of the LQRPA method to the low-lying states in $^{30,32,34}\text{Mg}$ (from [49]). (a) Collective potential $V(\beta, \gamma)$ for ^{30}Mg . The HFB equilibrium points are indicated by red circles. (b)–(d) Vibrational wave functions squared, $\sum_k |\Phi_{\alpha k}(\beta, \gamma)|^2$, of the 0_1^+ , 2_1^+ , and 0_2^+ states in ^{30}Mg . Contour lines are drawn at every tenth part of the maximum value. (e)–(h) and (i)–(l): same set of figures but for ^{32}Mg and ^{34}Mg , respectively.

A problem of the Inglis–Belyaev cranking formula is that time-odd mean-field effects are ignored and it underestimates the collective masses (inertial functions) [72]. Moving mean fields possess time-odd components that change sign under time reversal operation, but the cranking formula ignores their effects on the collective masses. By taking into account such time-odd corrections to the cranking masses, one can better reproduce low-lying spectra [53].

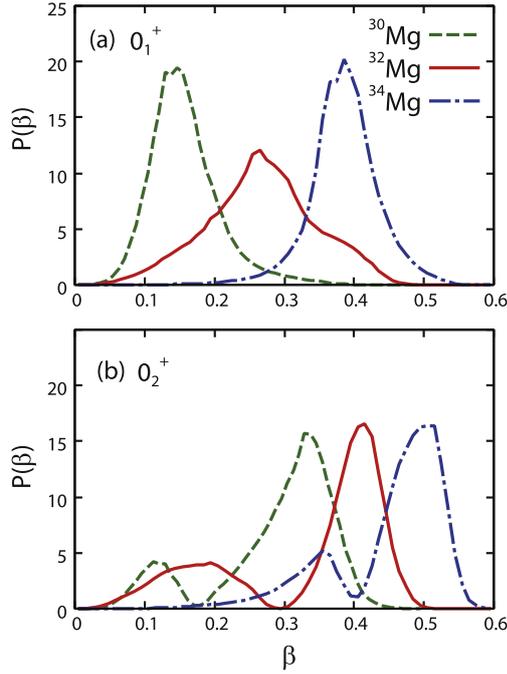


Figure 4. (a) Probability densities integrated over γ , $P(\beta) = \int d\gamma |\Phi_{\alpha I=0, K=0}(\beta, \gamma)|^2 |G(\beta, \gamma)|^{1/2}$, for the ground 0_1^+ states in $^{30,32,34}\text{Mg}$ plotted as functions of β (from [49]). (b) Same as (a) but for the excited 0_2^+ states.

5.2. Adiabatic TDHF theory

Attempts to self-consistently derive the collective Hamiltonian using adiabatic approximation to time evolution of mean fields started in 1960s [44, 73]. In these pioneer works, the collective quadrupole coordinates (β, γ) were defined in terms of expectation values of the quadrupole operators and the 5D collective Hamiltonian was derived using the P + Q force model [48]. During 1970s this approach was generalized to be applicable to any effective interaction. This advanced approach is called adiabatic TDHF (ATDHF) [74–76].

In the ATDHF theory, the density matrix $\rho(t)$ is written in the following form and expanded as a power series with respect to $\chi(t)$.

$$\rho(t) = e^{i\chi(t)} \rho_0(t) e^{-i\chi(t)} \quad (45)$$

$$= \rho_0(t) + i[\chi(t), \rho_0(t)] - \frac{1}{2}[\chi(t), [\chi(t), \rho_0(t)]] + \dots \quad (46)$$

Baranger and Vénéroni [74] suggested a possibility to introduce collective coordinates as parameters describing the time evolution of the density matrix $\rho_0(t)$ and discussed an iterative procedure to solve the ATDHF equations. But this idea has not been realized until now. We note that the ATDHF does not reduce to the RPA in the small-amplitude limit if a few collective coordinates are introduced by hand. In fact it gives a collective mass different from the RPA [77].

The ATDHF theory developed by Villars [78] aims at self-consistent determination of the optimum collective coordinates on the basis of the time-dependent variational principle. This approach, however, encountered a difficulty that we could not get unique solutions of its basic equations determining the collective path. This problem was later solved by treating the second-order terms of the momentum expansion in a self-consistent manner [37, 79]. It was shown that, when the number of collective coordinate is only one, a collective path maximally decoupled from non-collective degrees of freedom runs along a valley in the multi-dimensional potential-energy surface associated with the TDHF states.

To describe low-frequency collective motions, it is necessary to take into account the pairing correlations. In other words, we need to develop the adiabatic TDHFB (ATDHFB) theory. This is one of the reasons why applications of the ATDHF have been restricted to collective phenomena where pairing correlations play minor roles such as low-energy collisions between spherical closed-shell nuclei [80] and giant resonances [77]. When large-amplitude shape fluctuations take place, single-particle level crossings often occur. To follow the adiabatic configuration across the level crossing points, the pairing correlation plays an essential role. Thus, an extension to ATDHFB is indispensable for the description of low-frequency collective excitations.

In the past, Dobaczewski and Skalski [81] tried to develop the ATDHFB theory assuming the axially symmetric quadrupole deformation parameter β as the collective coordinate. Quite recently, Li *et al* [82] tried to derive the 5D quadrupole collective Hamiltonian on the basis of the ATDHFB. The extension of ATDHF to ATDHFB is not straightforward, however. This is because, as discussed in section 2, we need to decouple the number-fluctuation degrees of freedom from the LACM of interest and respect the gauge invariance with respect to the pairing rotational angles.

5.3. Boson expansion method

Boson expansion method is well known as a useful microscopic method of describing anharmonic (non-linear) vibrations going beyond the harmonic approximation of the QRPA. In this approach, we first construct a collective subspace spanned by many-phonon states of vibrational quanta (determined by the QRPA) in the huge-dimensional shell-model space, and then map these many-phonon states one-to-one to many-boson states in an ideal boson space. Anharmonic effects neglected in the QRPA are treated as higher-order terms in the power-series expansion with respect to the boson creation and annihilation operators. Starting from the QRPA about a spherical shape, one can thus derive the 5D quadrupole collective Hamiltonian in a fully quantum mechanical manner. The boson expansion method has been successfully applied to low-energy quadrupole excitation spectra in a wide range of nuclei including those lying in regions of quantum phase transitions from spherical to deformed [83, 84].

In the time-dependent mean-field picture, state vectors in the boson expansion method are written in terms of the creation and annihilation operators ($\Gamma_i^\dagger, \Gamma_i$) of the QRPA eigen-modes, or, equivalently, in terms of the collective coordinate and momentum operators (\hat{Q}_i, \hat{P}_i),

$$|\phi(t)\rangle = \exp \left[\sum_i (\eta_i(t) \Gamma_i^\dagger - \eta_i^*(t) \Gamma_i) \right] |\phi_0\rangle \quad (47)$$

$$= \exp \left[i \sum_i (p_i(t) \hat{Q}_i - q_i(t) \hat{P}_i) \right] |\phi_0\rangle. \quad (48)$$

With increasing amplitudes of the quadrupole shape vibration $|\eta_i(t)|$ (values of the collective coordinate $q_i(t)$), anharmonic (non-linear) effects become stronger. Strong non-linear effects may eventually change even the microscopic structure of the collective operators (\hat{Q}_i , \hat{P}_i) determined by the QRPA. In such situations, it is desirable to construct a theory that allows variations of microscopic structure of collective operators as functions of $q_i(t)$. It may be said that the SCC method has accomplished this task.

5.4. Generator coordinate method (GCM)

The GCM has been used for a wide variety of nuclear collective phenomena [85–87]. Using the angular-momentum projector \hat{P}_{IMK} and the neutron(proton)-number projector \hat{P}_N (\hat{P}_Z), we write the state vector as a superposition of the projected mean-field states with different deformation parameters (β, γ) ,

$$|\Psi_{NZIM}^i\rangle = \int d\beta d\gamma \sum_K f_{NZIK}^i(\beta, \gamma) \hat{P}_N \hat{P}_Z \hat{P}_{IMK} |\phi(\beta, \gamma)\rangle. \quad (49)$$

Because the projection operators contain integrations, it has been a difficult task to carry out such high-dimensional numerical integrations in solving the Hill–Wheeler equation for the states $|\phi(\beta, \gamma)\rangle$ obtained by the constrained HFB method. In recent years, however, remarkable progress has been taking place, which makes it possible to carry out such large-scale numerical computations [88–93]. The HFB calculations using the density dependent effective interactions are better founded by density functional theory (DFT). Accordingly, the modern GCM calculation is referred to as ‘multi-reference DFT’ [88].

It is well known that one can derive a collective Schrödinger equation by making a gaussian overlap approximation (GOA) to the Hill–Wheeler equation [94–96]. There is no guarantee, however, that dynamical effects associated with time-odd components of moving mean field are sufficiently taken into account in the collective masses (inertial functions) obtained through this procedure. In the case of center of mass motion, we need to use complex generator coordinates to obtain the correct mass, implying that collective momenta conjugate to collective coordinates should also be treated as generator coordinates [22, 97].

A fundamental question is how to choose the optimal generator coordinates. With the variational principle, Holzwarth and Yukawa [98] proved that the mean-field states parametrized by a single optimal generator coordinate run along a valley of the collective potential energy surface. This line of investigation was further developed [99] and greatly stimulated the challenge toward constructing a microscopic theory of LACM. In this connection, we note that conventional GCM calculations parametrized by a few real generator coordinates do not reduce to the QRPA in the small-amplitude limit, differently from the case that all two-quasiparticle (particle–hole) degrees of freedom are treated as complex generator coordinates [100].

It is very important to distinguish the 5D collective Hamiltonian obtained by making use of the GOA to the GCM from that derived in section 3 on the basis of the ASCC method. In the latter, the canonical conjugate pairs of collective coordinate and momentum are self-consistently derived on the basis of the time-dependent variational principle. The canonical formulation enables us to adopt the standard canonical quantization procedure. Furthermore, effects of the time-odd components of the moving mean field are automatically taken into account in the collective masses (inertial functions). In view of the above points, it is highly desirable to carry out a systematic comparison of collective inertial masses evaluated by different approximations including the ASCC, the ATDHFB, the GCM + GOA, and the adiabatic cranking methods for a better understanding of their physical implications. In this

connection, it is interesting to notice that the results of the recent GCM calculation for ^{76}Kr [92], using the particle-number and angular-momentum projected basis (49), are rather similar to those obtained by use of the 5D collective Hamiltonian with the Inglis–Belyaev cranking masses, except for an overall overestimation of the excitation energies by about 20%.

6. Challenges for future

As reviewed by Hyde and Wood [5], nature of low-lying excited 0^+ states, systematically found in recent experiments as well as those known from old days, is not well understood. It is thus quite challenging to apply, in a systematic ways, the 5D collective Hamiltonian approach to all of these data, from light to heavy and from stable to unstable nuclei, and explore the limit of its applicability. Recalling that the importance of the couplings between the quadrupole and pairing vibrations has been pointed out [14–16], one of the basic questions is ‘under what situations we need to extend the 5D collective Hamiltonian to 7D by explicitly treating the proton and neutron pairing gaps as dynamical variables.’

Another interesting subject is to extend the collective Hamiltonian approach to a variety of collective phenomena, for example, those observed in rapidly rotating nuclei, heavy and super heavy nuclei, neutron-rich unstable nuclei, by taking into account the effects of rapid rotation and/or continuum, from the beginning in the single-particle (HFB) Hamiltonian. Macroscopic quantum tunnelings through self-consistently generated barriers, such as spontaneous fissions and deep sub-barrier fusions, are, needless to say, longstanding yet modern, fundamental subjects of nuclear structure physics.

It is a great challenge to develop the CHF + LQRPA approach on the basis of the time-dependent DFT. To efficiently solve the large-dimensional LQRPA equations containing density-dependent terms, the finite-amplitude method recently developed in [101–104] may be utilized.

Acknowledgments

This work is supported by the JSPS KAKENHI Grant No. 25287065. One of the authors (KS) is supported by the Special Postdoctoral Researcher Program of RIKEN.

References

- [1] Bohr A and Mottelson B R 1975 *Nuclear Structure* vol 2 (New York: Benjamin) (World Scientific, 1998)
- [2] Åberg S, Flocard H and Nazarewicz W 1990 *Annu. Rev. Nucl. Part. Sci.* **40** 439
- [3] Bender M, Heenen P-H and Reinhard P-G 2003 *Rev. Mod. Phys.* **75** 121
- [4] Rowe D J and Wood J L 2010 *Fundamentals of nuclear models Foundational Models* (Singapore: World Scientific)
- [5] Heyde K and Wood J L 2011 *Rev. Mod. Phys.* **83** 1467
- [6] Anderson P W 1958 *Phys. Rev.* **112** 1900
Anderson P W 1963 *Phys. Rev.* **130** 439
- [7] Nambu Y 1960 *Phys. Rev.* **117** 648
- [8] Brink D M and Broglia R A 2005 *Nuclear Superfluidity, Pairing in Finite Systems* (Cambridge: Cambridge University Press)
- [9] Frauendorf S 2001 *Rev. Mod. Phys.* **73** 463
- [10] Bohr A 1976 *Rev. Mod. Phys.* **48** 365
- [11] Mottelson B 1976 *Rev. Mod. Phys.* **48** 375
- [12] Próchniak L and Rohoziński S G 2009 *J. Phys. G: Nucl. Part. Phys.* **36** 123101

- [13] Matsuo M and Matsuyanagi K 1985 *Prog. Theor. Phys.* **74** 1227
Matsuo M and Matsuyanagi K 1986 *Prog. Theor. Phys.* **76** 93
Matsuo M and Matsuyanagi K 1987 *Prog. Theor. Phys.* **78** 591
- [14] Iwasaki S, Marumori T, Sakata F and Takada K 1976 *Prog. Theor. Phys.* **56** 1140
- [15] Weeks K J, Tamura T, Udagawa T and Hahne F J W 1981 *Phys. Rev. C* **24** 703
- [16] Takada K and Tazaki S 1986 *Nucl. Phys. A* **448** 56
- [17] Negele J W 1982 *Rev. Mod. Phys.* **54** 913
- [18] Abe A and Suzuki T (ed) 1983 Microscopic theories of nuclear collective motions *Prog. Theor. Phys. Suppl.* **74 & 75** 1–416
- [19] Yamamura M and Kuriyama A 1987 *Prog. Theor. Phys. Suppl.* **93** 1–175
- [20] Kuriyama A, Matsuyanagi K, Sakata F, Takada K and Yamamura M (ed) 2001 Selected topics in the Boson mapping and time-dependent Hartree-Fock methods *Prog. Theor. Phys. Suppl.* **141** 1
- [21] Nakatsukasa T, Walet N R and do Dang G 1999 *Phys. Rev. C* **61** 014302
- [22] Ring P and Schuck P 1980 *The Nuclear Many-Body Problem* (Berlin: Springer)
- [23] Blaizot J-P and Ripka G 1986 *Quantum Theory of Finite Systems* (Cambridge, MA: MIT Press)
- [24] Matsuyanagi K, Matsuo M, Nakatsukasa T, Hinohara N and Sato K 2010 *J. Phys. G: Nucl. Part. Phys.* **37** 064018
- [25] Nakatsukasa T 2012 *Prog. Theor. Exp. Phys.* **2012** 01A207
- [26] Matsuyanagi K, Hinohara N and Sato K 2013 *Fifty Years of Nuclear BCS: Pairing in Finite Systems* (Singapore: World Scientific)
- [27] Rowe D J and Bassermann R 1976 *Can. J. Phys.* **54** 1941
- [28] Marumori T 1977 *Prog. Theor. Phys.* **57** 112
- [29] Marumori T, Maskawa T, Sakata F and Kuriyama A 1980 *Prog. Theor. Phys.* **64** 1294
- [30] Rowe D J 1982 *Nucl. Phys.* **391** 307
- [31] Matsuo M 1986 *Prog. Theor. Phys.* **76** 372
- [32] Matsuo M and Matsuyanagi K 1985 *Prog. Theor. Phys.* **74** 288
- [33] Matsuo M, Shimizu Y R and Matsuyanagi K 1985 *Proc. Niels Bohr Centennial Conf. Nuclear Structure (North-Holland)* ed R Broglia *et al* p 161
- [34] Yamada K 1993 *Prog. Theor. Phys.* **89** 995
- [35] Shimizu Y R and Matsuyanagi K 2001 *Prog. Theor. Phys. Suppl.* **141** 285
- [36] Matsuo M, Nakatsukasa T and Matsuyanagi K 2000 *Prog. Theor. Phys.* **103** 959
- [37] Klein A, Walet N R and do Dang G 1991 *Ann. Phys.* **208** 90
- [38] Almeded D and Walet N R 2004 *Phys. Rev. C* **69** 024302
- [39] Barranco F, Bertsch G F, Broglia R A and Vigezzi E 1990 *Nucl. Phys. A* **512** 253
- [40] Hinohara N, Nakatsukasa T, Matsuo M and Matsuyanagi K 2007 *Prog. Theor. Phys.* **117** 451
- [41] Hinohara N, Sato K, Nakatsukasa T, Matsuo M and Matsuyanagi K 2010 *Phys. Rev. C* **82** 064313
- [42] Sato K and Hinohara N 2011 *Nucl. Phys. A* **849** 53
- [43] Sato K, Hinohara N, Yoshida K, Nakatsukasa T, Matsuo M and Matsuyanagi K 2012 *Phys. Rev. C* **86** 024316
- [44] Baranger M and Kumar K 1965 *Nucl. Phys.* **62** 113
Baranger M and Kumar K 1968 *Nucl. Phys. A* **110** 529
Baranger M and Kumar K 1968 *Nucl. Phys. A* **122** 241
Baranger M and Kumar K 1968 *Nucl. Phys. A* **122** 273
- [45] Thouless D J and Valatin J G 1962 *Nucl. Phys.* **31** 211
- [46] Eisenberg J M and Greiner W 1987 *Nuclear Theory* vol 1 3rd edn (Amsterdam: North Holland)
- [47] Kumar K and Baranger M 1967 *Nucl. Phys.* **92** 608
- [48] Bes D R and Sorensen R A 1969 *Advances in Nuclear Physics* vol 2 (New York: Plenum) p 129
- [49] Hinohara N, Sato K, Nakatsukasa T, Matsuo M and Matsuyanagi K 2011 *Phys. Rev. C* **84** 061302(R)
- [50] Yoshida K and Hinohara N 2011 *Phys. Rev. C* **83** 061302(R)
- [51] Hinohara N, Nakatsukasa T, Matsuo M and Matsuyanagi K 2009 *Phys. Rev. C* **80** 014305
- [52] Hinohara N and Kanada-En'yo Y 2011 *Phys. Rev. C* **83** 014321
- [53] Hinohara N, Li Z P, Nakatsukasa T, Nikšić T and Vretenar D 2012 *Phys. Rev. C* **85** 024323
- [54] Fischer S M *et al* 2003 *Phys. Rev. C* **67** 064318
- [55] Iwasaki H *et al* 2014 *Phys. Rev. Lett.* **112** 142502
- [56] Hamamoto I 2012 *Phys. Rev. C* **85** 064329

- [57] Wimmer K *et al* 2010 *Phys. Rev. Lett.* **105** 252501
- [58] do Dang G, Klein A and Walet N R 2000 *Phys. Rep.* **335** 93
- [59] Brack M, Damgaard J, Jensen A S, Pauli H C, Strutinsky V M and Wong C Y 1972 *Rev. Mod. Phys.* **44** 320
- [60] Baran A, Sheikh J A, Dobaczewski J, Nazarewicz W and Staszczak A 2011 *Phys. Rev. C* **84** 054321
- [61] Libert J, Girod M and Delaroche J-P 1999 *Phys. Rev. C* **60** 054301
- [62] Yuldashbaeva E Kh, Libert J, Quentin P and Girod M 1999 *Phys. Lett. B* **461** 1
- [63] Próchniak L, Quentin P, Samsøen D and Libert J 2004 *Nucl. Phys. A* **730** 59
- [64] Delaroche J-P, Girod M, Libert J, Goutte H, Hilaire S, Péru S, Pillet N and Bertsch G F 2010 *Phys. Rev. C* **81** 014303
- [65] Nikšić T, Li Z P, Vretenar D, Próchniak L, Meng J and Ring P 2009 *Phys. Rev. C* **79** 034303
- [66] Li Z P, Nikšić T, Vretenar D, Meng J, Lalazissis G A and Ring P 2009 *Phys. Rev. C* **79** 054301
- [67] Li Z P, Nikšić T, Vretenar D and Meng J 2010 *Phys. Rev. C* **81** 034316
- [68] Li Z P, Nikšić T, Vretenar D, Ring P and Meng J 2010 *Phys. Rev. C* **81** 064321
- [69] Li Z P, Yao J M, Vretenar D, Nikšić T, Chen H and Meng J 2011 *Phys. Rev. C* **84** 054304
- [70] Nikšić T, Vretenar D and Ring P 2011 *Prog. Part. Nucl. Phys.* **66** 519
- [71] Fu Y, Mei H, Xiang J, Li Z P, Yao J M and Meng J 2013 *Phys. Rev. C* **87** 054305
- [72] Dobaczewski J and Dudek J 1995 *Phys. Rev. C* **52** 1827
- [73] Belyaev S T 1965 *Nucl. Phys.* **64** 17
- [74] Baranger M and Vénéroni M 1978 *Ann. Phys.* **114** 123
- [75] Brink D M, Giannoni M J and Veneroni M 1976 *Nucl. Phys. A* **258** 237
- [76] Goeke K and Reinhard P-G 1978 *Ann. Phys.* **112** 328
- [77] Giannoni M J and Quentin P 1980 *Phys. Rev. C* **21** 2060
- Giannoni M J and Quentin P 1980 *Phys. Rev. C* **21** 2076
- [78] Villars F 1977 *Nucl. Phys. A* **285** 269
- [79] Mukherjee A K and Pal M K 1982 *Nucl. Phys. A* **373** 289
- [80] Goeke K, Cusson R Y, Grummer F, Reinhard P-G and Reinhardt H 1983 *Prog. Theor. Phys. Suppl.* **74 & 75** 33
- [81] Dobaczewski J and Skalski J 1981 *Nucl. Phys. A* **369** 123
- [82] Li Z P, Nikšić T, Ring P, Vretenar D, Yao J M and Meng J 2012 *Phys. Rev. C* **86** 034334
- [83] Sakamoto H and Kishimoto T 1988 *Nucl. Phys. A* **486** 1
- Sakamoto H and Kishimoto T 1991 *Nucl. Phys. A* **528** 73
- [84] Klein A and Marshalek E R 1991 *Rev. Mod. Phys.* **63** 375
- [85] Reinhard P-G and Goeke K 1987 *Rep. Prog. Phys.* **50** 1
- [86] Egido J L and Robledo L M 2004 *Extended Density Functionals in Nuclear Physics (Lecture Notes in Physics vol 641)* ed G A Lalazissis *et al* (Berlin: Springer) p 269
- [87] Bender M 2008 *Eur. Phys. J. Spec. Top.* **156** 217
- [88] Bender M and Heenen P-H 2008 *Phys. Rev. C* **78** 024309
- [89] Rodríguez T R and Egido J L 2010 *Phys. Rev. C* **81** 064323
- [90] Yao J M, Meng J, Ring P and Vretenar D 2010 *Phys. Rev. C* **81** 044311
- [91] Yao J M, Mei H, Chen H, Meng J, Ring P and Vretenar D 2011 *Phys. Rev. C* **83** 014308
- [92] Yao J M, Hagino K, Li Z P, Meng J and Ring P 2014 *Phys. Rev. C* **89** 054306
- [93] Rodríguez T R 2014 *Phys. Rev. C* **90** 034306
- [94] Griffin J J and Wheeler J A 1957 *Phys. Rev.* **108** 311
- [95] Onishi N and Une T 1975 *Prog. Theor. Phys.* **53** 504
- [96] Rohoziński S G 2012 *J. Phys. G: Nucl. Part. Phys.* **39** 095104
- [97] Peierls R E and Thouless D J 1962 *Nucl. Phys.* **38** 154
- [98] Holzwarth G and Yukawa T 1974 *Nucl. Phys. A* **219** 125
- [99] Reinhard P-G and Goeke K 1979 *Phys. Rev. C* **20** 1546
- [100] Jancovici B and Schiff D H 1964 *Nucl. Phys.* **58** 678
- [101] Nakatsukasa T, Inakura T and Yabana K 2007 *Phys. Rev. C* **76** 024318
- [102] Avogadro P and Nakatsukasa T 2011 *Phys. Rev. C* **84** 014314
- [103] Avogadro P and Nakatsukasa T 2013 *Phys. Rev. C* **87** 014331
- [104] Hinojara N, Kortelainen M and Nazarewicz W 2013 *Phys. Rev. C* **87** 064309