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THE BOHR HAMILTONIAN: A PURE QUANTUM PROCEDURE*

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Dedicated to Professor Krzysztof Pomorski on the occasion of the 50th anniversary of his scientific activity

The Generating Coordinate Method applied to the description of the collective quadrupole states of both the even- and the odd-particle nuclei is resumed. The five laboratory components of the spherical quadrupole tensor are taken as the generator coordinates. Use of the method for the even and the odd systems is confronted with regard to the conservation of the time-reversal symmetry. The adiabatic approximation for the overlaps of the generating functions in the case of systems with the conserved and the broken time-reversal symmetry is formulated. In that approximation, the Hill–Wheeler equations can be substituted by the one second-order differential equation in the case of the time-even nuclei, and by the system of the two coupled second-order differential equations in the case of those with the broken time-reversal symmetry. In the former case, the new formulae for the weight, the inertial functions and moments of inertia, and the potential of the Bohr Hamiltonian were obtained. In the latter one, the new approach to the description of the collective quadrupole states of the odd nuclei was formulated.

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1. Introduction

The original idea of the Bohr Hamiltonian comes obviously from the classical physics. The multipole vibrations of the spherical drop of incompressible liquid [1] were prototypes for the nuclear collective excitations. The quantum description of nuclear collective states was initiated by Bohr [2] who

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quantized the Rayleigh liquid-drop vibrations. The original Bohr Hamiltonian was simply the harmonic oscillator. It initiated the era of the collective-Hamiltonian models for various types of nuclei. Here, we shall not be interested in the phenomenological models for the collective Hamiltonians. We are going to discuss the derivations of the Bohr Hamiltonian from microscopic many-body theories. The method of derivation, which is used up to now, was proposed by Belyaev [3] and, independently, by Kumar and Baranger [4]. The method have consisted in the construction of the general, five-dimensional (in the case of the quadrupole coordinates) *classical* Hamiltonian with the coordinate-dependent mass parameters. The all functions of coordinates, which define the Hamiltonian, have been extracted from the given microscopic theory using the Adiabatic Time Dependent Hartree– Fock(–Bogolyubov)-type of method (ATDHFB). Finally, the Hamiltonian has been quantized by the Podolsky–Pauli prescription [5–7] and used in the following form:

$$H(\boldsymbol{\alpha}) = -\frac{1}{2\sqrt{B(\boldsymbol{\alpha})}} \frac{\partial}{\partial \alpha_{\mu}} \sqrt{B(\boldsymbol{\alpha})} B_{\mu\nu}^{-1}(\boldsymbol{\alpha}) \frac{\partial}{\partial \alpha_{\nu}} + V(\boldsymbol{\alpha}), \qquad (1.1)$$

where α is the tensor of the collective coordinates, $B_{\mu\nu}$ is the inertial bitensor and B is the determinant of it. (The summation convention for the upper and lower indices is used throughout the paper.) Different microscopic theories are applied to the description of the collective states. However, the quasi-classical method of construction of the Hamiltonian is still used. Needless to say that the Bohr-Hamiltonian approach applies to the even-even nuclear systems only.

Yet, it turns out that a pure quantum procedure can be given which leads to the differential eigenvalue equation for the collective states, that is to say, to the Bohr Hamiltonian. It is already formulated [8, 9] but not very well known and still does not applied to calculations of collective states. Therefore, the method will be recapitulated here with paying the special attention to its quantum nature, and to similarities and differences between the even and the odd nuclear systems. Maybe, the present paper will contribute to popularization of the approach.

2. Generating the quadrupole collective states

Let a nuclear system be described by the microscopic many-body Hamiltonian \hat{H} , which is supposed to be invariant under the time reversal \hat{T} and rotations $\hat{R}(\omega)$ in the physical three-dimensional space. The simplest and the best known approximations of the many-body Hamiltonian are these of the mean-field type. The variational Generator Coordinate Method (GCM) will be used to generate the collective states from the constraint mean-field eigenstates $|\phi(q)\rangle$ called the intrinsic states. The tacit assumption is that we deal with the ground states. For the collective quadrupole states, the constraint is the condition that the two intrinsic components of the ground-state mass quadrupole moment take the given values $q = (q_0, q_2)$. The intrinsic components of the quadrupole moment together with the three Euler angles $\omega = (\varphi, \vartheta, \psi)$ of the orientation of the intrisic axes (principal axes of the quadrupole moment tensor) with respect to the laboratory frame will be used as the generator coordinates. Instead, it is more convenient to use the five laboratory components $\alpha_{\mu}(\omega, q)$ ($\alpha^{\mu} = (-1)^{\mu}\alpha_{-\mu}$) of the quadrupole tensor $\boldsymbol{\alpha}$. The states $|\phi(q)\rangle$ rotated to the laboratory frame, namely

$$|\Phi(\boldsymbol{\alpha})\rangle = \hat{R}(\omega)|\phi(q)\rangle \tag{2.1}$$

will serve as the generating states. It could seem that the method applies to the nuclear systems with an arbitrary number of the (quasi-)particles. However, it is not so, because the intrinsic states $|\phi(q)\rangle$ for the even and the odd number of particles have some different features.

The intrinsic state $|\phi(q)\rangle \equiv |\phi_{\rm e}(q)\rangle$ of the even systems is invariant under the time reversal and we have

$$\hat{T}|\phi_{\rm e}(q)\rangle = |\phi_{\rm e}(q)\rangle.$$
 (2.2)

In consequence, the matrix elements of the Hermitian operators between both the intrinsic and the laboratory states are real and symmetric.

The intrisic states of odd systems, $|\phi(q)\rangle \equiv |\phi_{o}(q)\rangle$ appear in the degenerate Kramers doublets, time-reversed to one another, $|\phi_{o}(q)\rangle$ and $|\bar{\phi}_{o}(q)\rangle$, such that

$$\left|\bar{\phi}_{\rm o}(q)\right\rangle = \hat{T}\left|\phi_{\rm o}(q)\right\rangle \tag{2.3}$$

which means that the time-reversal symmetry is broken. We construct them in such a way that they are both eigenstates of the *T*-signature, \hat{R}_y^T with the eigenvalue equal to 1. Both states in the Kramers doublet, rotated to the laboratory frame, have to be treated as the generating states. The matrix elements between these states are complex in general.

The trial states in the GCM for the even and the odd systems should be obviously different. The trial state for the even nuclei is assumed in the following form:

$$|\Psi_{\rm e}[\varphi]\rangle = \int \varphi(\alpha) |\Phi_{\rm e}(\alpha)\rangle \mathrm{d}\Omega(\alpha),$$
 (2.4)

where $\varphi(\boldsymbol{\alpha})$ is the weight function. The variational principle leads to the Hill–Wheeler integral equation [10] of the form of

$$\int \left[\mathcal{H}_{e} \left(\boldsymbol{\alpha}, \boldsymbol{\alpha}' \right) - E \mathcal{I}_{e} \left(\boldsymbol{\alpha}, \boldsymbol{\alpha}' \right) \right] \varphi \left(\boldsymbol{\alpha}' \right) d\Omega \left(\boldsymbol{\alpha}' \right) = 0, \qquad (2.5)$$

where the overlap and the energy kernels are the following:

$$\mathcal{I}_{e}(\boldsymbol{\alpha}, \boldsymbol{\alpha}') = \left\langle \Phi_{e}(\boldsymbol{\alpha}) \middle| \Phi_{e}(\boldsymbol{\alpha}') \right\rangle$$
(2.6)

and

$$\mathcal{H}_{\mathrm{e}}\left(\boldsymbol{\alpha},\boldsymbol{\alpha}'\right) = \left\langle \Phi_{\mathrm{e}}(\boldsymbol{\alpha}) \middle| \hat{H} \middle| \Phi_{\mathrm{e}}\left(\boldsymbol{\alpha}'\right) \right\rangle \,, \tag{2.7}$$

respectively. Both kernels are real symmetric.

The case of the odd systems is more complicated. The trial state is a functional of the two weight functions, namely

$$|\Psi_{\rm o}[\varphi,\bar{\varphi}]\rangle = \int \left[\varphi(\boldsymbol{\alpha}) \left| \Phi_{\rm o}(\boldsymbol{\alpha}) \right\rangle + \bar{\varphi}(\boldsymbol{\alpha}) \left| \bar{\Phi}_{\rm o}(\boldsymbol{\alpha}) \right\rangle \right] \mathrm{d}\Omega(\boldsymbol{\alpha}) \,. \tag{2.8}$$

In consequence, the variational principle leads to the two coupled integral equations of the following form:

$$\int \left[\begin{pmatrix} \mathcal{H}_{o}(\boldsymbol{\alpha},\boldsymbol{\alpha}'), & -\bar{\mathcal{H}}_{o}^{*}(\boldsymbol{\alpha},\boldsymbol{\alpha}') \\ \bar{\mathcal{H}}_{o}(\boldsymbol{\alpha},\boldsymbol{\alpha}'), & \mathcal{H}_{o}^{*}(\boldsymbol{\alpha},\boldsymbol{\alpha}') \end{pmatrix} - E \begin{pmatrix} \mathcal{I}_{o}(\boldsymbol{\alpha},\boldsymbol{\alpha}'), & -\bar{\mathcal{I}}_{o}^{*}(\boldsymbol{\alpha},\boldsymbol{\alpha}') \\ \bar{\mathcal{I}}_{o}(\boldsymbol{\alpha},\boldsymbol{\alpha}'), & \mathcal{I}_{o}^{*}(\boldsymbol{\alpha},\boldsymbol{\alpha}') \end{pmatrix} \right] \begin{pmatrix} \varphi(\boldsymbol{\alpha}') \\ \bar{\varphi}(\boldsymbol{\alpha}') \end{pmatrix} d\Omega(\boldsymbol{\alpha}') = 0, \quad (2.9)$$

where the twinned and mixed overlap and energy kernels are the following:

$$\mathcal{I}_{o}(\boldsymbol{\alpha},\boldsymbol{\alpha}') = \left\langle \Phi_{o}(\boldsymbol{\alpha}) \middle| \Phi_{o}(\boldsymbol{\alpha}') \right\rangle, \quad \bar{\mathcal{I}}_{o}(\boldsymbol{\alpha},\boldsymbol{\alpha}') = \left\langle \bar{\Phi}_{o}(\boldsymbol{\alpha}) \middle| \Phi_{o}(\boldsymbol{\alpha}') \right\rangle, \quad (2.10)$$

and

$$\mathcal{H}_{o}(\boldsymbol{\alpha},\boldsymbol{\alpha}') = \left\langle \Phi_{o}(\boldsymbol{\alpha}) \middle| \hat{H} \middle| \Phi_{o}(\boldsymbol{\alpha}') \right\rangle, \quad \bar{\mathcal{H}}_{o}(\boldsymbol{\alpha},\boldsymbol{\alpha}') = \left\langle \bar{\Phi}_{o}(\boldsymbol{\alpha}) \middle| \hat{H} \middle| \Phi_{o}(\boldsymbol{\alpha}') \right\rangle h$$
(2.11)

respectively. All these kernels are, in general, complex. The twinned kernels are Hermitian, whereas the mixed ones are anti-symmetric.

3. The adiabatic approximation

The kernels in the Hill–Wheeler integral equations (2.5) and (2.9) can be calculated when the many-body Hamiltonian \hat{H} and its mean-field eigenstates $|\phi(q)\rangle$ are known. They express the complicated structure of the many-body states. The adiabatic approximation consists in the negligence of that structure. It means that we approximate the kernels by means of the smooth functions which have the expected behavior and properties. In the case of the even systems, the overlap kernels are symmetric, real, positive everywhere and tend asymptoticly to zero. Therefore, we approximate the overlap kernel by the Gaussian function, namely

$$\mathcal{I}_{e}\left(\boldsymbol{\beta} + \frac{1}{2}\boldsymbol{\gamma}, \boldsymbol{\beta} - \frac{1}{2}\boldsymbol{\gamma}\right) \approx \exp\left(-\frac{1}{2}g^{\mu\nu}(\boldsymbol{\beta})\gamma_{\mu}\gamma_{\nu}\right),\tag{3.1}$$

where $\beta = \frac{1}{2}(\alpha + \alpha')$ and $\gamma = \alpha - \alpha'$ (the summation convention for upper and lower indexes is used) with

$$g^{\mu\nu}(\boldsymbol{\beta}) = -\frac{\partial^2 \mathcal{I}_{\rm e}(\boldsymbol{\beta}, \boldsymbol{\beta})}{\partial \gamma_{\mu} \partial \gamma_{\nu}} \,. \tag{3.2}$$

Matrix \mathbf{g} is real, symmetric and positive definite. The approximation is known within the GCM [11] and called Gaussian Overlap Approximation (GOA). The energy kernel contains additionally the quadratic term, namely

$$\mathcal{H}_{e}\left(\boldsymbol{\beta} + \frac{1}{2}\boldsymbol{\gamma}, \boldsymbol{\beta} - \frac{1}{2}\boldsymbol{\gamma}\right) = \exp\left(-\frac{1}{2}g^{\mu\nu}(\boldsymbol{\beta})\gamma_{\mu}\gamma_{\nu}\right)\left[v(\boldsymbol{\beta}) - \frac{1}{2}h^{\mu\nu}(\boldsymbol{\beta})\gamma_{\mu}\gamma_{\nu}\right]$$
(3.3)

with

$$v(\boldsymbol{\beta}) = \mathcal{H}_{e}(\boldsymbol{\beta}, \boldsymbol{\beta}),$$

$$h^{\mu\nu}(\boldsymbol{\beta}) = -\frac{\partial^{2}\mathcal{H}_{e}(\boldsymbol{\beta}, \boldsymbol{\beta})}{\partial\gamma_{\mu}\partial\gamma_{\nu}} - g^{\mu\nu}(\boldsymbol{\beta})v(\boldsymbol{\beta}). \qquad (3.4)$$

Matrix h is real and symmetric as well.

In the case of the odd systems, we have to go beyond the GOA, because the kernels are not real. The twinned kernels are Hermitian. Therefore, we supplement the exponent in the counterpart of Eq. (3.1) with the imaginary term, linear in γ , namely

$$\mathcal{I}_{o}\left(\boldsymbol{\beta}+\frac{1}{2}\boldsymbol{\gamma},\boldsymbol{\beta}-\frac{1}{2}\boldsymbol{\gamma}\right) = \exp\left(ik^{\mu}(\boldsymbol{\beta})\gamma_{\mu}-\frac{1}{2}g^{\mu\nu}(\boldsymbol{\beta})\gamma_{\mu}\gamma_{\nu}\right),\qquad(3.5)$$

where

$$k^{\mu}(\boldsymbol{\beta}) = -i \frac{\partial \mathcal{I}_{o}(\boldsymbol{\beta}, \boldsymbol{\beta})}{\partial \gamma_{\mu}} \,. \tag{3.6}$$

The counterpart of Eq. (3.3) takes the following form:

$$\mathcal{H}_{o}\left(\boldsymbol{\beta} + \frac{1}{2}\boldsymbol{\gamma}, \boldsymbol{\beta} - \frac{1}{2}\boldsymbol{\gamma}\right) = \mathcal{I}_{o}\left(\boldsymbol{\beta} + \frac{1}{2}\boldsymbol{\gamma}, \boldsymbol{\beta} - \frac{1}{2}\boldsymbol{\gamma}\right)\left[\boldsymbol{v}(\boldsymbol{\beta}) + i\boldsymbol{u}^{\mu}(\boldsymbol{\beta})\boldsymbol{\gamma}_{\mu} - \frac{1}{2}\boldsymbol{h}^{\mu\nu}(\boldsymbol{\beta})\boldsymbol{\gamma}_{\mu}\boldsymbol{\gamma}_{\nu}\right] \quad (3.7)$$

with

$$u^{\mu}(\boldsymbol{\beta}) = -i\frac{\partial}{\partial\gamma_{\mu}} \left(\frac{\mathcal{H}_{o}(\boldsymbol{\beta},\boldsymbol{\beta})}{\mathcal{I}_{o}(\boldsymbol{\beta},\boldsymbol{\beta})}\right).$$
(3.8)

The mixed kernels are anti-symmetric and can be presented in the form of matrix elements of the anti-Hermitian operator \hat{R}_y^T within twinned generating states. For instance,

$$\bar{\mathcal{I}}_{o}\left(\boldsymbol{\alpha},\boldsymbol{\alpha}'\right) = \left\langle \Phi_{o}(\tilde{\boldsymbol{\alpha}}) \right| \hat{R}_{y}^{T} \left| \Phi_{o}\left(\boldsymbol{\alpha}'\right) \right\rangle \,, \tag{3.9}$$

where

$$\tilde{\alpha}_{\mu} = \sum_{\nu} \mathcal{D}^2_{\mu\nu}(0,\pi,0)\alpha_{\nu} \tag{3.10}$$

is the quadrupole tensor α rotated around the intrinsic *y*-axis by angle π . Hence, the mixed overlap and energy kernels can be presented within the adiabatic approximation as follows:

$$\bar{\mathcal{I}}_{o}\left(\boldsymbol{\alpha},\boldsymbol{\alpha}'\right) = \mathcal{I}_{o}\left(\tilde{\boldsymbol{\alpha}},\boldsymbol{\alpha}'\right)\bar{f}^{\mu}(\boldsymbol{\beta})\gamma_{\mu}$$
(3.11)

and

$$\bar{\mathcal{H}}_{o}(\boldsymbol{\alpha},\boldsymbol{\alpha}') = \mathcal{I}_{o}(\tilde{\boldsymbol{\alpha}},\boldsymbol{\alpha}') \bar{u}^{\mu}(\boldsymbol{\beta})\gamma_{\mu}, \qquad (3.12)$$

respectively, where

$$\bar{f}^{\mu}(\boldsymbol{\beta}) = \frac{\partial}{\partial \gamma_{\mu}} \left(\frac{\bar{\mathcal{I}}_{o}(\boldsymbol{\alpha}, \boldsymbol{\alpha}')}{\mathcal{I}_{o}(\tilde{\boldsymbol{\alpha}}, \boldsymbol{\alpha}')} \right)$$
(3.13)

and

$$\bar{u}^{\mu}(\boldsymbol{\beta}) = \frac{\partial}{\partial \gamma_{\mu}} \left(\frac{\mathcal{H}_{o}(\boldsymbol{\alpha}, \boldsymbol{\alpha}')}{\mathcal{I}_{o}(\tilde{\boldsymbol{\alpha}}, \boldsymbol{\alpha}')} \right) \,. \tag{3.14}$$

4. The Bohr Hamiltonians

It has been known for a long time that the one-dimensional Hill–Wheeler integral equation (2.5) with the GOA kernels, Eqs. (3.1) and (3.3), can be approximated by the second-order differential equation [11]. It was shown [12, 13] that it is still true in the case of several generator coordinates. In that case, a tacit assumption is that the space of the generator coordinates with the metric tensor **g** is flat. Using the Fourier analysis of the Gaussian energy kernel, Onishi and Une [14] showed that the Hill–Wheeler integral equation is formally equivalent to the differential equation having the Schrödinger-type form.

We applied the GCM with the GOA to generate the quadrupole collective states of the time-even nuclear systems [8]. We chose the five laboratory components of the quadrupole tensor $\boldsymbol{\alpha}$ as the generating coordinates in spite of the common opinion that the three Euler angles $\omega = \varphi, \vartheta, \psi$ and the two intrinsic components of the quadrupole tensor q_0 , q_2 should play the role of them. We derived the Schrödinger equation

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$$H_{\rm e}\psi(\boldsymbol{\alpha}) = E\psi(\boldsymbol{\alpha}) \tag{4.1}$$

from the Hill–Wheeler equation (2.5) with the Gaussian kernels. The wave function ψ is defined as follows:

$$\psi(\boldsymbol{\alpha}) = \int \mathcal{R}(\boldsymbol{\alpha}, \boldsymbol{\alpha}') \varphi(\boldsymbol{\alpha}') d\Omega(\boldsymbol{\alpha}') , \qquad (4.2)$$

where the square-root kernel

$$\mathcal{R}(\boldsymbol{\alpha},\boldsymbol{\xi}) = \left(\frac{2}{\pi}\right)^{5/4} \exp\left(-g^{\mu\nu}\left(\frac{1}{2}(\boldsymbol{\xi}+\boldsymbol{\alpha})\right)(\boldsymbol{\xi}_{\mu}-\boldsymbol{\alpha}_{\mu})(\boldsymbol{\xi}_{\nu}-\boldsymbol{\alpha}_{\nu})\right) \quad (4.3)$$

is such that

$$\int \mathcal{R}(\boldsymbol{\alpha}, \boldsymbol{\xi}) \mathcal{R}\left(\boldsymbol{\xi}, \boldsymbol{\alpha}'\right) \sqrt{g(\boldsymbol{\xi})} \mathrm{d}\Omega((\boldsymbol{\xi}))$$
$$= \exp\left(-\frac{1}{2}g^{\mu\nu} \left(\frac{1}{2} \left(\boldsymbol{\alpha} + \boldsymbol{\alpha}'\right)\right) \left(\alpha_{\mu} - \alpha'_{\mu}\right) \left(\alpha_{\nu} - \alpha'_{\nu}\right)\right)$$
(4.4)

and $g(\boldsymbol{\xi}) = \det \mathbf{g}(\boldsymbol{\xi})$. The Bohr Hamiltonian has the following form:

$$H_{\rm e} = -\frac{1}{2\sqrt{g(\boldsymbol{\alpha})}} \frac{\partial}{\partial \alpha_{\mu}} \sqrt{g(\boldsymbol{\alpha})} A_{\mu\nu}(\boldsymbol{\alpha}) \frac{\partial}{\partial \alpha_{\nu}} + V(\boldsymbol{\alpha}) \,. \tag{4.5}$$

We have called it the Bohr Hamiltonian despite it has the weight $\sqrt{g(\alpha)}$ which is different from the weight $\sqrt{B(\alpha)}$ ($A \equiv B^{-1}$) of the Hamiltonian of Eq. (1.1). Such a difference between the quasi-classical and quantum Hamiltonians was foreseen already in [15]. It is still one more important hidden difference between the quantum and the quasi-classical Hamiltonian. The potential $V(\alpha)$ in Eq. (4.5) contains the so-called zero-point energy corrections of the quantum origin which never appear in the quasi-classical static potentials (Eq. (1.1)). The Bohr Hamiltonian H of Eq. (1.1) is valid for the even-particle systems because they may have their classical counterparts. The Hamiltonian H_e of Eq. (4.5) is valid for the even-particle systems because they are time-even.

In the case of the odd systems, we try to approximate the system of the two Hill–Wheeler integral equations (2.9) with the adiabatic kernels (3.5), (3.7), and (3.9), (3.12) by the system of the differential equations. The problem is more complicated than that in the even systems not only because of the two weight functions, $\varphi(\alpha)$ and $\bar{\varphi}(\alpha)$ forming the alispinor, instead of the single scalar one. In the present case, the adiabatic approximation is not exactly the GOA. Moreover, we deal with the two quadrupole tensors, α and

 $\tilde{\alpha}$ (dependent on each other — see Eq. (3.10)). Therefore, the methods used in Refs. [11–13] should be modified. It was done in Ref. [9]. In consequence, we obtain the following generalized eigenvalue differential equation in the so-called alispin space:

$$\begin{bmatrix} \begin{pmatrix} H_{o}(\boldsymbol{\alpha}), & -\bar{H_{o}}^{\dagger}(\boldsymbol{\alpha}) \\ \bar{H_{o}}(\boldsymbol{\alpha}), & H_{o}^{*}(\boldsymbol{\alpha}) \end{bmatrix} - E \begin{pmatrix} 1, & -\bar{N_{o}}^{\dagger}(\boldsymbol{\alpha}) \\ \bar{N_{o}}(\boldsymbol{\alpha}), & 1 \end{bmatrix} \begin{bmatrix} \psi(\boldsymbol{\alpha}) \\ \bar{\psi}(\boldsymbol{\alpha}) \end{bmatrix} = 0.$$
(4.6)

Relation between the alispinor wave function and the alispinor weight function is the following:

$$\begin{pmatrix} \psi(\boldsymbol{\alpha}) \\ \bar{\psi}(\boldsymbol{\alpha}) \end{pmatrix} = \exp\left(i\boldsymbol{k}(\boldsymbol{\alpha})\cdot\boldsymbol{\alpha}\right) \left(\int_{\mathcal{R}}^{\mathcal{R}}(\boldsymbol{\alpha},\boldsymbol{\alpha}')\exp\left(-i\boldsymbol{k}(\boldsymbol{\alpha}')\cdot\boldsymbol{\alpha}'\right)\varphi\left(\boldsymbol{\alpha}'\right)\mathrm{d}\Omega\left(\boldsymbol{\alpha}'\right) \\ \int_{\mathcal{R}}^{\mathcal{R}}(\boldsymbol{\alpha},\tilde{\boldsymbol{\alpha}}')\exp\left(-i\boldsymbol{k}\left(\tilde{\boldsymbol{\alpha}}'\right)\cdot\tilde{\boldsymbol{\alpha}}'\right)\bar{\varphi}\left(\boldsymbol{\alpha}'\right)\mathrm{d}\Omega\left(\boldsymbol{\alpha}'\right) \right)$$
(4.7)

(see Eq. (4.3) for the definition of the square-root kernel \mathcal{R}). The two diagonal elements of the Hamiltonian matrix are the differential operators, $H_{\rm o}$ and $H_{\rm o}^*$, time-reversed to each other. The former one has the following form:

$$H_{o}(\boldsymbol{\alpha}) = -\frac{1}{2\sqrt{g(\boldsymbol{\alpha})}} \frac{\partial}{\partial \alpha_{\mu}} \sqrt{g(\boldsymbol{\alpha})} A_{\mu\nu}(\boldsymbol{\alpha}) \frac{\partial}{\partial \alpha_{\nu}} -i\frac{1}{2\sqrt{g(\boldsymbol{\alpha})}} \left(\frac{\partial}{\partial \alpha_{\mu}} \sqrt{g(\boldsymbol{\alpha})} U_{\mu}(\boldsymbol{\alpha}) + \sqrt{g(\boldsymbol{\alpha})} U_{\mu}(\boldsymbol{\alpha}) \frac{\partial}{\partial \alpha_{\mu}} \right) + V(\boldsymbol{\alpha}) .$$
(4.8)

In comparison to the Bohr Hamiltonian, $H_{\rm e}$, of Eq. (4.5), it contains the imaginary term with the first order differential operator. This is due to the time-reversal symmetry breaking, which is the case for the odd systems. Therefore, the Hamiltonian of Eq. (4.8) is called the Bohr Hamiltonian for the odd systems. The non-diagonal elements in the Hamiltonian and norm matrices are the first-order differential operators and take the following forms:

$$\bar{H}_{o}(\boldsymbol{\alpha}) = -\frac{1}{2\sqrt{g(\boldsymbol{\alpha})}} \left(\frac{\partial}{\partial \tilde{\alpha}_{\mu}} \sqrt{g(\boldsymbol{\alpha})} \bar{U}_{\mu}(\boldsymbol{\alpha}) + \sqrt{g(\boldsymbol{\alpha})} \bar{U}_{\mu}(\boldsymbol{\alpha}) \frac{\partial}{\partial \alpha_{\mu}} \right) + \bar{u}^{\mu}(\boldsymbol{\alpha}) (\tilde{\alpha}_{\mu} - \alpha_{\mu})$$
(4.9)

and

$$\bar{N}_{o}(\boldsymbol{\alpha}) = -\frac{1}{2\sqrt{g(\boldsymbol{\alpha})}} \left(\frac{\partial}{\partial \tilde{\alpha}_{\mu}} \sqrt{g(\boldsymbol{\alpha})} \bar{F}_{2\mu}(\boldsymbol{\alpha}) + \sqrt{g(\boldsymbol{\alpha})} \bar{F}_{\mu}(\boldsymbol{\alpha}) \frac{\partial}{\partial \alpha_{\mu}} \right) + \bar{f}^{\mu}(\boldsymbol{\alpha}) (\tilde{\alpha}_{\mu} - \alpha_{\mu}), \qquad (4.10)$$

respectively.

Using the laboratory components α_{μ} of the quadrupole tensor as the generator coordinates has the great advantage. Due to that we obtained the five-dimensional differential equations, Eqs. (4.1) and (4.6), which allow us to describe the most general quadrupole excitations of the even and the odd nuclear systems, respectively. Nobody has been succeeded in deriving the general five-dimensional quantum Bohr Hamiltonian using the intrinsic coordinates: the Euler angles $\omega = (\varphi, \vartheta, \psi)$ and intrinsic quadrupole moments $q = (q_0, q_2)$. However, the transformation to the intrinsic frame is required when solving the five-dimensional equations. Then the Euler angles appear in the equations in the form of the three differential angular momentum operators, $L_x(\omega)$, $L_y(\omega)$, $L_z(\omega)$, which have the known eigenfunctions $\mathcal{D}^I_{MK}(\omega)$ (see Ref. [15]). The remaining quantities, which appear in the equations, are functions of the two intrinsic quadrupole moments, q_0 , q_2 . In consequence, we are left with the systems of the two-dimensional differential equations to solve.

5. Conclusions

We recapitulated our investigations on the nuclear collective quadrupole states by means of the quantum variational Generator Coordinate Method (GCM). Here, we discussed the principal assumptions and the most important results. All the details of the derivations and all the formulae useful for the calculations are contained in Refs. [8, 9]. To investigate the quadrupole excitations, the laboratory components of the quadrupole tensor were chosen as the five generator coordinates. It is well-known that the variational principle leads to the Hill–Wheeler integral equations. However, it turned out that in the approximation, which we call adiabatic, the integral equations can be substituted by the second-order differential equations in the five-dimensional space. In spite of the uniform approach for the all nuclear systems, there are the essential differences in the treatment of the even- and the odd-particle nuclei. The time-reversal symmetry is the clue.

Equation (2.2) shows that the time-reversal symmetry is conserved in the even-particle systems. Then, the overlaps of the generating states are real positive and the adiabatic approximation is simply the GOA. In such a case, the Hill–Wheeler equation reduces to the second-order differential equation with the real, Hermitian Hamiltonian. The structure of this Hamiltonian is identical with that of the quasi-classical Bohr Hamiltonian, and this is why the procedure of solving the eigenvalue equation (4.1) is known. A few computational codes diagonalizing the Bohr Hamiltonians are at the public disposal on the market (*e.g.*, Ref. [16]). The formulae for the weight, the three inertial functions, the three moments of inertia and the potential can be taken from Ref. [8] to diagonalize the new Bohr Hamiltonian. It would be interesting whether the results will be different, better or worse, to those obtained so far with the quasi-classical approaches.

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Another story is with the odd systems. Equation (2.3) indicates breaking of the time-reversal symmetry. The generating states are associated automatically in the Kramers doublets and the number of the Hill–Wheeler equations has doubled. The notion of the alispinors arises. The overlaps are, in general, complex. The adiabatic approximation should be extended beyond the GOA. Finally, the two Hill–Wheeler equations in the alispin space can be approximated by the doublet of the coupled second-order differential equations. On the contrary to equation (4.1) in the case of the even nuclei, the alispinor equations (4.6) for the odd systems are quite new and not known commonly. No procedures for solving them have been developed. The collective models for the odd nuclei have dealt with the systems core(s) plus (quasi-)particle and have coped with the doubtful phenomenon of the core polarization. Here, we treat the odd nucleus as a whole and no core polarization appears. It would be worthwhile to develop such a new approach to the odd nuclei.

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