Microscopic description of collective properties of even-even Xe isotopes

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Abstract

The collective properties of even-even $^{118-144}$Xe isotopes have been studied within a model that uses the general Bohr Hamiltonian derived from the mean-field theory based on the UNEDF0 energy functional. The calculated low-energy spectra and E2 transition probabilities are in good agreement with the experimental data.

Keywords: collective model, mean-field theory, ATDHFB method, general Bohr Hamiltonian, energy density functional

1. Introduction

Currently developed mean-field theories based on energy density functionals ambitiously aim to properly explain a wide range of nuclear properties, and in many fields they have been quite successful. In this paper, I present the results of applying the UNEDF0 functional [1] to describe low-energy collective excitations in the chain of even-even $^{118-144}$Xe isotopes. The treatment of collective properties is based on the adiabatic time-dependent Hartree–Fock–Bogolyubov (HFB) (ATDHFB) theory, which leads to the construction of a collective Hamiltonian from a microscopic mean-field input. More details of the applied methods can be found in [2, 3]. An alternative approach to collective phenomena within a microscopic theory with phenomenological interactions employs the generator coordinate method, as seen in [4–6]. One should also mention an attempt to describe collective phenomena in the random phase approximation context, starting from realistic interactions and using the unitary correlation operator method [7, 8].

For many years Xe nuclei have been the subject of extensive experimental and theoretical study. Many of these studies focused on the phenomenon of the double $\beta$ decay (confirmed experimentally in the case of $^{136}$Xe), but there is also extensive literature concerning the collective properties related to changes in nuclear deformation. The long chain of Xe isotopes offers a good opportunity to study the evolution of these properties as the number of neutrons increases, and also to study the role of nonaxiality. Let me mention a few works that studied one or more of the even-even Xe isotopes: papers employing geometrical concepts and the Bohr Hamiltonian [2, 9–12], papers based on the interacting boson model [13–16], and papers using truncated shell model space [17–19].

Section 2 presents some basic facts on the general Bohr Hamiltonian (GBH), on the methods that allow for its derivation from the mean-field theory, and on the UNEDF0 density energy functional. In section 3, I show the results of calculations concerning several low-spin energy levels, some E2 transitions in the $^{118-144}$Xe nuclei, and comparisons with experimental data.

2. Theory

2.1. Quadrupole variables, the Bohr Hamiltonian

A consistent description of nuclear vibrational and rotational excitations and of possible couplings between them requires the use of quadrupole collective variables (i.e., of the second rank with respect to the SO(3) rotation group). These variables can be chosen in various ways, including as parameters describing the shape of a nucleus [20, 21] or the shape of a phenomenological one-particle potential [9, 10, 22]. Within a self-consistent mean-field theory such quadrupole variables, $\alpha_\mu$ (in the laboratory frame), are chosen to be proportional to the components of the quadrupole mass tensor

$$\alpha_\mu \sim \left\langle \Phi \left| \sum_{i=1}^A e^2 Y_{2\mu}(\theta_i, \phi_i) \right| \Phi \right\rangle$$

where $\Phi$ is a microscopic nuclear wave function that can be...
obtained by using effective interactions of the Skyrme [2] or the Gogny type [23, 24] or in the relativistic framework [25, 26]. The quadrupole variables can be equivalently expressed in the intrinsic frame (also called the principal axes frame) by two deformation variables, $\beta$, $\gamma$, and three Euler angles ($\Omega$) describing the relative orientation of the laboratory and intrinsic frame. The $\beta$, $\gamma$ variables are given by the mean values of the operators, $Q_0 = \sum_{i=1}^{A} (z_i^2 - r_i^2)$ and $Q_2 = \sum_{i=1}^{A} \sqrt{3} (x_i^2 - y_i^2)$, as follows

$$
\beta \cos \gamma = c q_0, \quad q_0 = \langle \Phi | Q_0 | \Phi \rangle \quad (2)
$$

$$
\beta \sin \gamma = c q_2, \quad q_2 = \langle \Phi | Q_2 | \Phi \rangle \quad (3)
$$

with a conventional factor, $c = \sqrt{\pi/5}/Ar^2$, where $r^2 = 3/5r_0^2 A^{2/3}$, $r_0 = 1.2$ fm.

One should keep in mind that in some theoretical approaches (e.g., in the geometrical collective (Frankfurt model [27])), the deformation variables, $\beta$, $\gamma$, do not have a direct relation to a nuclear shape or mass distribution. Within the framework of the interacting boson model [28], the $\beta$, $\gamma$ variables introduced by means of the so-called coherent states are instead related with properties of valence nucleons, and not of the spatial distribution of a nuclear density.

The general properties of the quadrupole collective space, as well as of functions and operators depending on the quadrupole variables, can be found in [3]. The most important operator, from the point of view of physical applications, is a Hamiltonian that we call the GBH, which can be expressed in the intrinsic frame as

$$
H_{\text{Bohr}} = T_{\text{vib}} + T_{\text{rot}} + V \quad (4)
$$

$$
T_{\text{vib}} = -\frac{1}{2\sqrt{\hbar}} \left\{ \frac{1}{\beta^4} \left[ \frac{\partial}{\partial \beta} \left( \frac{\beta^4}{\sqrt{\hbar}} B_{\rho \beta} \right) \right] \partial \beta \right. \\
- \left. \frac{1}{\beta^2} \left[ \frac{\partial}{\partial \beta} \left( \frac{\beta^3}{\sqrt{\hbar}} B_{\rho \beta} \right) \right] \partial \gamma \right\} \\
+ \frac{1}{\beta \sin 3\gamma} \left[ \frac{\partial}{\partial \beta} \left( \frac{\beta^3}{\sqrt{\hbar}} \sin 3\gamma B_{\rho \beta} \right) \right] \partial \gamma \\
+ \frac{1}{\beta^2} \left[ \frac{\partial}{\partial \beta} \left( \frac{\beta^3}{\sqrt{\hbar}} \sin 3\gamma B_{\rho \beta} \right) \right] \partial \gamma
$$

$$
T_{\text{rot}} = \frac{1}{2} \sum_{k=1}^{A} \left( \Omega_k^2 / J_k \right) J_k = 4B_k (\beta, \gamma) \beta^2 \sin^2(\gamma - 2\pi k/3) \quad (6)
$$

$$
\text{where} \quad w = B_{\rho \beta} B_{\gamma \gamma} - B_{\rho \gamma} ; \quad r = B_1 B_2 B_3. \quad (7)
$$

The operators, $J_k(\Omega)$, $k = 1, 2, 3$, are components of the angular momentum in the intrinsic frame. The Hamiltonian (4) contains seven functions that depend on deformation variables: the potential energy, $V$, and six functions, $B_{\rho \beta}$, $B_{\rho \gamma}$, $B_{\gamma \gamma}$, $B_1$, $B_2$, $B_3$, called mass parameters or inertial functions. One possible way to determine these seven functions consists in assuming for them a ‘reasonable’ form, with some free parameters that are determined through comparison of the calculated and experimental collective properties. I use another approach, which is based on the ATDHFB theory and which aims at calculating these functions, starting from a microscopic theory. In this approach, one does not introduce any additional free parameters, and the prediction of the collective properties is based solely on the knowledge of effective nucleon-nucleon interactions.

### 2.2. The ATDHFB mass parameters

In the following discussion, it is assumed that the time evolution of a system is determined through the time dependence of several collective variables, $q_i$ (not necessarily the quadrupole ones from equations (2) and (3)). The ATDHFB theory, based on an assumption of low collective velocities, gives an expression, $\frac{1}{2} \sum_{k,j} b_{ij} q_i q_j$, which is bilinear in velocities and which defines a metric tensor in the collective space. In the next step, this expression is used to calculate the Laplace–Beltrami operator, which is taken (up to the $\hbar^2$ factor) as the kinetic energy part of a collective Hamiltonian. Functions $b_{ij}$ (mass parameters) depend on collective variables. More details on the ATDHFB theory and mass parameters can be found in [3, 29] and papers cited therein. Below, I briefly sketch some steps and give some formulas that are needed to calculate the GBH, starting from the UNEDF0 energy functional.

The so-called cranking approximation ignores the Thouless–Valatin terms, so that the mass parameters can be conveniently expressed through derivatives of a generalized density matrix, $R(q)$, corresponding to the HFB state, $\Phi(q)$. The derivative, $\partial \Phi(R)$, in the quasiparticle basis (in the doubled space) has the form

$$
\left( \frac{\partial}{\partial q_k} R \right)_{\text{quasipart}} = F_k = \begin{pmatrix} 0 & f_k \\ f_k & 0 \end{pmatrix}, \quad \dot{f}_k = -f_k^* \quad (8)
$$

and the mass parameters read

$$
b_{ij} = \frac{\hbar^2}{2} \sum_{\mu \nu} f_{\mu \nu}^* f_{\nu \mu} + f_{\mu \nu}^* f_{\nu \mu} \quad (9)
$$

where $E_{\mu \nu}$ are quasiparticle energies. If the matrix $\partial \Phi(R)$ is known in a fixed single-particle basis, the matrix $F_k$ can be calculated as

$$
F_k = B \left( \partial \Phi(R) \right)_{\text{fixed,doubled}} B^+ \quad (10)
$$

where $B$ is the Bogolyubov matrix for $R$

$$
B = \begin{pmatrix} U^+ & V^* \\ V & U^T \end{pmatrix} \quad (11)
$$

Sometimes the following alternative expression for $f_k$ is useful

$$
f_{\mu \nu} = \langle \Phi | a_{\mu} a_{\nu} | \partial \Phi \rangle \quad (12)
$$

where $\alpha_{\mu \nu}$ are quasiparticle annihilation operators.

In the case of quadrupole variables, one obtains the deformation-dependent HFB state by constrained HFB
calculations
\[ \delta \langle \Phi | H_{\text{micro}} | \Phi \rangle = 0 \quad \text{with} \quad \langle \Phi | Q_j | \Phi \rangle = q_j, \]
\[ j = 0, 2. \]

Then, it is easier to first discuss the vibrational mass parameters, \( B_{\beta \beta}, \beta = 0, 2 \), from which \( B_{\gamma \gamma}, B_{\beta \gamma}, B_{\gamma \beta} \) in formulas (5)–(7) can be calculated by a simple change of variables. The required derivatives, \( \partial R/\partial \lambda_j \), should be calculated by numerical differentiation (see [2, 29, 30]), but most often one resorts to another (so-called perturbative) approximation, which relates the derivatives of the generalized density matrix to derivatives of the induced one-body Hamiltonian [3]. The constraints (equation (13)) lead to the extra term, \( -\lambda_j Q_{\mu} \), in the induced one-body Hamiltonian, and one can easily calculate a derivative with respect to \( \lambda_j \):
\[ f_j = \frac{1}{E_\mu + E_\nu} (w_j)_{\mu \nu}, \]
\[ w_j = U^+(Q)_{\text{fixed}} V^\ast - \left( U^+(Q)_{\text{fixed}} V^\ast \right)^T. \]

Then, the derivatives, \( \partial h/R \), are calculated using the relation
\[ \frac{\partial}{\partial q_k} = \sum_{j} \frac{\partial h}{\partial \lambda_j} \frac{\partial \lambda_j}{\partial q_k} \]
and finally the derivatives, \( \partial h/q \), are obtained by inverting the matrix \( \partial h/q \), which can also be expressed through \( w_j \) from equation (15)
\[ \frac{\partial h}{\partial \lambda_j} = \text{Re} \sum_{\mu \nu} \left( \frac{w_j}{E_\mu + E_\nu} \right)_{\mu \nu}. \]

The moments of inertia are given by the Inglis–Belyaev formula
\[ J_k = \sum_{\mu \nu} \left( \frac{U^+(j_k)_{\text{fixed}} V^\ast - \left( U^+(j_k)_{\text{fixed}} V^\ast \right)^T}{E_\mu + E_\nu} \right)_{\mu \nu}. \]

The Lipkin–Nogami (LN) method is used to avoid the pairing ‘collapse’ for magic nuclei and their neighbors. The pairing strengths for protons and neutrons, \( V^p_{0,\mu} \), are fitted simultaneously with other parameters determining the functional. A truncation of the quasiparticle space, required due to the zero-range of the pairing interaction, is fixed by the condition for quasiparticle energies, \( E_\mu < 60 \text{ MeV} \). Because it is well known that the ATDHFB mass parameters are quite sensitive to the diffuseness of the occupation number distribution, I will now present more details on the treatment of the pairing part of UNEDF0.

Figure 1. Plot of the pairing energy (upper panel) and of the effective pairing gap, \( \Delta_\mu + \lambda_{2,\mu} \), calculated for protons (●) and neutrons (○) at the deformation corresponding to a minimum of the potential energy.

The binding energies of the considered Xe isotopes are reproduced quite well by the UNEDF0 functional. The root mean square deviation (RMSD) for 16 nuclei is equal to 0.454 MeV, with the largest error, \( B_{\text{th}} - B_{\text{exp}} = -0.71 \text{ MeV} \), for the \(^{136}\text{Xe} \) isotope. The chain of isotopes contains \(^{136}\text{Xe} \) with a magic number, \( N = 82 \), of neutrons, but it appears that due to the LN prescription, the changes of the pairing properties along the chain are quite smooth. This can be seen in Figure 1, where I plot the neutron and proton pairing energy versus the mass number. In addition, I show a plot of the quantity, \( \Delta_\mu + \lambda_{2,\mu} \), where \( \Delta_\mu = \sum_{\mu_\mu} \lambda_\mu / \sum_{\mu_\mu} \mu_\mu \) and \( \lambda_{2,\mu} \) is a coefficient determined with the LN method. This quantity can be treated as an estimation of the pairing gap within the LN method; for more details, see [34].
In conclusion, I want to mention two newer functionals, UNEDF1 [35] and UNEDF2 [35, 36], which were constructed by extending the empirical dataset used in the fitting procedure. In the case of the UNEDF1 functional, new data on a few fission isomers were added, while for the UNEDF2, several single-particle level splittings were additionally considered. However, the RMSD for the binding energies is significantly lower (around 1.4 MeV) for UNEDF0 than it is for UNEDF1 and UNEDF2 (around 1.9 MeV). Hence, the UNEDF0 functional seems to be a good choice for a pilot study of collective properties in the region of medium-heavy nuclei. A further detailed study on the consequences of UNEDF1 and UNEDF2 for collective nuclear properties is currently in progress.

3. Results of calculations, comparison with experiment

The values of inertial functions and potential energy that enter the GBH were calculated at 144 points, forming a regular grid in the sextant \(0 \leq \beta \leq 0.65 \times 0 \leq \gamma \leq 60^\circ\) in the deformation plane. The distance between the points is 0.05 and 6° in the \(\beta\) and \(\gamma\) directions, respectively. The mean-field wave functions were obtained using the code HFODD ver. 2.49t; see [37] and references therein.

3.1. Potential energy surfaces

As one can see in figure 2, there are three nuclei, \(^{134-138}\text{Xe}\), with a spherical minimum of the potential energy. Others exhibit deformed minima with \(\beta_{\text{min}}\) in the range 0.1–0.25, mostly on the prolate axis, except for \(^{118}\text{Xe}\) and \(^{128}\text{Xe}\), which have slightly nonaxial minima with \(\gamma_{\text{min}} = 8^\circ\) and 12°, respectively. The depths of the minima (relative to a spherical shape) are less than 2 MeV. In figures 3 and 4, I show full plots of the potential energy on the deformation space for a representative sample of four isotopes. One can see a rather weak dependence of the potential energy on the \(\gamma\) variable (\(\gamma\) softness), especially for lighter isotopes.

3.2. Collective energy levels

Having calculated the potential energy and mass parameters, I performed a numerical diagonalization of the resulting Bohr Hamiltonian using the method described in [2, 10]. The obtained eigenvalues can be directly compared with the excited energy levels of positive parity, and the corresponding collective wave functions can be then used to calculate the matrix elements of various operators, in particular of the operators of electromagnetic E2 transitions.

I should add that all mass parameters (vibrational and rotational) were multiplied before the diagonalization of the Bohr Hamiltonian by a constant factor of 1.3. The commonly quoted reasons for introducing such a factor refer to simulating the effects of including the Thouless–Valatin terms in the ATDHFB method and/or the effects of the so-called pairing vibrations [2, 3, 23, 38, 39]. Some rather crude estimations of these effects give the value of the factor in the range of 1.2–1.5. However, due to a lack of sufficiently quantitative calculations, this factor must be treated as an additional parameter of the theory. Before presenting the results for the whole chain of Xe isotopes, I will show the consequences of introducing the scaling factor for energy spectra and B(E2) probabilities in the case of \(^{136}\text{Xe}\). Figure 5 contains plots of bands built on \(0_1\), \(2_2\), and \(0_2\) levels. There are two sets of theoretical results, obtained both with the scaling factor (sc = 1.3) and without the scaling factor (sc = 1). One can see that the scaling produces a ‘shrinking’ of the spectra, leaving a general picture that is similar in both cases. In addition, one can see that the scaling leads to a better agreement with experimental data (shown in figure 5 as well).

![Figure 2](image-url)

**Figure 2.** (a) Value of the deformation \(\beta_{\text{min}}\) (left panel) and \(\gamma_{\text{min}}\) (right panel) at the minimum of the potential energy. (b) Depth (relative to a value at a spherical shape) of minima of the potential energy for the \(^{114-144}\text{Xe}\) nuclei.
A sample of $B(E2)$ results (theoretical with and without scaling and experimental) is shown in figure 6. The sample contains cases with both good and worse agreement between theory and experiment. One can see that the effect of the scaling on the mass parameters is much smaller on the $B(E2)$ probabilities than on the values of level energies.

Then I compare theoretical energies of several low-lying low-spin levels ($2_1^+, 4_1^+, 2_2^+, 0_1^+, 0_2^+$) with experimental data [40] for the considered chain of Xe isotopes. These levels were chosen because of their role in analyzing the band structure of nuclear spectra.

One can conclude from the plots in figures 7–11 that in general, the theoretical results are in good agreement with the experimental data, especially for the lighter part of the isotope chain (up to $A = 130$). One should also keep in mind that I do not fit any parameters to collective properties. Some
significant discrepancies in the vicinity of the \( N = 82 \) number of neutrons are not unexpected because the ATDHF theory tends to perform better for more collective nuclei (i.e. with a larger number of valence nucleons; let us recall that there are only four valence protons in Xe isotopes). This effect is connected with an assumption of the adiabatic motion of all nucleons in the varying mean field. This assumption is strongly affected by the presence of closed shells.

### 3.3. E2 transitions

A detailed analysis of the experimental data on electromagnetic transitions can provide important information about excited levels; see [41]. In the case of quadrupole excitations, the most important are E2 transitions, which are described by the collective operator

\[
Q^{(\text{charge})}_{\text{ad}} (\beta, \gamma) = \langle \Phi (\beta, \gamma) | e \sum_{\nu=1}^{2} r_{\nu}^2 Y_2^{\nu} (\theta, \phi) | \Phi (\beta, \gamma) \rangle. \tag{20}
\]

In figures 12 and 13, I present the results of calculations of the B(E2) reduced-transition probabilities for transitions \( 2^+_1 \rightarrow 0^+_1 \) and \( 4^+_1 \rightarrow 2^+_1 \), as well as their comparisons with evaluated experimental data from [40]. Again one can see that theoretical calculations reproduce the general behavior of B(E2) quite well, even though no free parameters (e.g. effective charges) were used.

In the case of some Xe isotopes, there are much more extensive experimental data on E2 transitions (see, [16] for \(^{126}\)Xe and [42, 43] for \(^{128}\)Xe), but I will leave a discussion of them for a subsequent publication.
4. Conclusions

The paper presented the results of the first attempt to apply the UNEDF0 energy functional to the theory of a nuclear collective motion. A correct description of the properties of the long chain of Xe isotopes considered is a demanding challenge to the theory, in particular to the framework with no free parameters that could be fitted to experimental data on collective levels. It can be argued that the results shown in section 3 are quite satisfactory and do a good job of reproducing the general tendencies seen in the energy spectra, as well as the E2 transitions in the Xe isotopes, with some exceptions around the semimagic $^{136}$Xe isotope. This contribution contains only a part of the obtained theoretical results, and a more detailed analysis of the $^{120-128}$Xe nuclei is in preparation.

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