Low-lying quadrupole collective states of the light and medium Xenon isotopes

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Abstract

Collective low lying levels of light and medium Xenon isotopes are deduced from the Generalized Bohr Hamiltonian (GBH). The microscopic seven functions entering into the GBH are built from a deformed mean field of the Woods-Saxon type. Theoretical spectra are found to be close to the ones of the experimental data taking into account that the calculations are completely microscopic, that is to say, without any fitting of parameters.

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I. INTRODUCTION:

The so-called General Bohr Hamiltonian (GBH) is applied to the light-medium even-even Xenon isotopes region $112 < A < 126$. This region lies between very deficient neutron nuclei with half-lives of few seconds and stable nuclei ($A = 124, 126$). The lightest isotopes ($A = 112 − 116$) are not very far away from the drip line (exotic nuclei) and hence experimental data such as band sequences and probability transitions are difficult to obtain. For these nuclei, we can find some data in Ref. [1]-[3]. Data of other isotopes ($A = 120 − 126$) are given in Ref.[6]-[13]. Some simple properties can easily be deduced from the concept of the equilibrium deformation. In effect, these isotopes have a proton number ($Z = 54$) which is somewhat close to the magic number of a closed shell ($Z = 50$) and thereby should not contribute to an effective deformation. However, the number of neutrons ($N = 58 − 72$) is far from closed shells ($N = 50$ or $82$), since the shape of the nucleus is due to both kinds of nucleons we finally should expect an appreciable deformation for these nuclei. Experiment corroborates that because quadrupole-beta values are found to be within the interval $0.19 < \beta < 0.29$. The most deformed nuclei are the isotopes $^{118−122}\text{Xenon}$ with a quadrupole deformation $\beta$ about $0.26 \sim 0.29$. These nuclei correspond to the neutron mid-shell region ($N = 64 \sim 66$). An other common interesting characteristic of these nuclei is the experimental ratio of the energy levels $R_{\text{exp}} = E(4_1)/E(2_1)$ which is about $2.3 \sim 2.5$ for all these isotopes. This means that these nuclei must belong to the shape-phase transitional region between the vibrational limit $R_{\text{exp}} = 2$ and the $\gamma$-unstable limit $R_{\text{exp}} = 2.5$.

There are a number of theoretical models that attempt to explain the collective states of the nuclei. The two main categories of these approaches are:

1. The GBH or geometrical model (see the next section) which treats the even-even nucleus as a quantal liquid drop which vibrates and rotates with coupling effects. It is a five dimensional Hamiltonian in which two collective variables are devoted to the vibrations of the nucleus and three Euler angles are used to specify its orientation with respect to the lab system. Basically it describes the dynamic of the quadrupole deformations of the nucleus but sometimes octupole or higher multipole orders are also considered. Some other models such a rovibrational model (RVM) can be assimilated to a particular case of the GBH model.

2. The interacting boson model (IBM) or algebraic model which assimilates the even-even nucleus to some bosons outside the closed shells. These bosons are of type d or s and are made of two nucleons strongly linked by the pairing interaction. For odd nuclei the IBM model is replaced by the interacting bosons-fermions approximation. In fact there are two versions for this model. In the IBM1, neutrons and protons are considered as the same bosons whereas in the IBM2 these kind of particles are considered as distinct. IBM models can be understood only from the group theory and the Lie algebra. Symmetries play a major role in this model. In the IBM1 model the vibrational, rotational and $\gamma$-soft (or $\gamma$-unstable nuclei) limits correspond respectively to the so-called $SU(5), U(3)$ and $SO(6)$ symmetries. Unlike the GBH, the IBM has a good number of particles (bosons).

All these approaches contain a certain number of parameters which can be considered as free and therefore can be fitted to experimental data to obtain the best possible results. But these parameters can also be derived from a microscopic theory. This is a reason why it has no sense to compare models in which parameters are fitted to experiment data with others that are based on pure microscopic approaches. In our case the GBH model contains seven parameters or more exactly seven functions. Apart from the macroscopic-microscopic method which is used to obtain the collective potential energy, the other six functions are evaluated on the basis of pure microscopic models. Similar calculations (but not exactly the same) have already been made in the past [15]-[19].

II. THE GBH MODEL

Historically the Bohr Hamiltonian was established as a phenomenological model to interpret harmonic vibrational and rotational spectra of the nuclei. Nowadays, the term "Bohr Hamiltonian" is commonly attributed to several similar collective hamiltonians. In this respect, we cite Ref. [14]. "The present-day notion of the Bohr Hamiltonian is not very precise. It encompasses a large class of Hamiltonians of which the original Bohr Hamiltonian is only a very special case [13]-[28]. Here, the GBH means a generic second-order differential Hermitian operator in the Hilbert space of functions of quadrupole coordinates. It is the most general collective Hamiltonian using the quadrupole coordinates. Making some natural assumptions [14], it is able to treat large amplitude collective motion. The main advantage of the GBH over the IBM model is coming from the fact that it can be derived from a microscopic theory. Two methods are usually used to this end: (1) The adiabatic time dependent Hartree-Fock-Bogoliubov method (ATDHFB) which leads to quantize with some ambiguities a classical Hamiltonian and (2) The Gaussian overlap approximation method associated with the generator coordinates method (GOA+GCM) which gives straightforwardly the quantum collective Hamiltonian. Both methods can be applied to different microscopic models such as the mean fields models based on
the Nilsson, Woods-Saxon potentials or even self-consistent calculations with Skyrme or Gogny effective interaction.

In this work we deal with the Generalized Bohr Hamiltonian defined as a sum of three operators:

$$H_{\text{col}} = T_{\text{vib}}(\beta, \gamma) + T_{\text{rot}}(\beta, \gamma, \theta_1, \theta_2, \theta_3) + U_{\text{col}}(\beta, \gamma)$$

where the kinetic vibrational energy and the kinetic rotational energy are given by [13]:

$$T_{\text{vib}}(\beta, \gamma) = -\frac{h^2}{2 \sqrt{wr}} \beta^T \left[ \frac{\partial}{\partial \beta} \left( \beta^T \sum_k B_{\beta\gamma} \frac{\partial}{\partial \beta} \right) \right]$$

$$+ \frac{\beta \sin(3\gamma)}{\sqrt{w}} \left[ -\frac{\partial}{\partial \gamma} \left( \sum_k \frac{\sin(3\gamma) B_{\beta\gamma}}{w} \frac{\partial}{\partial \beta} \right) + \frac{1}{\beta} \frac{\partial}{\partial \gamma} \left( \sum_k \frac{\sin(3\gamma) B_{\beta\gamma}}{w} \frac{\partial}{\partial \beta} \right) \right]$$

$$T_{\text{rot}}(\beta, \gamma, \Omega) = \frac{1}{2} \sum_{k=1,2,3} I_k^2(\theta_1, \theta_2, \theta_3)$$

Whereas the collective potential energy $U_{\text{col}}$ of the nucleus is defined as the potential energy of deformation of the nucleus (see the following section): $r$ and $w$ are given by: $w = B_{\beta\beta} B_{\gamma\gamma} - B_{\beta\gamma}^2$, $r = 3_1 3_2 3_3$

As already mentioned the GBH is a five dimensional Hamiltonian and hence contains five collective variables ($\beta, \gamma, \theta_1, \theta_2, \theta_3$). The GBH includes seven functions: The collective energy of deformation $U_{\text{col}}(\beta, \gamma)$, the three mass parameters $B_{\beta\beta}, B_{\beta\gamma}, B_{\gamma\gamma}$ and the three moments of inertia $3_1, 3_2, 3_3$ with respect to the principal axes. All these functions are deformation dependent.

The eigenvalues problem of the GBH has usual the form:

$$H_{\text{col}} \Psi_{\text{col}} = E_{\text{col}} \Psi_{\text{col}}$$

Analytical solutions of the Bohr Hamiltonian can be found in some remarkable cases of potentials: (1) the gamma unstable nuclei, (2) the harmonic oscillator potential, (3) the symmetric rotor model. These cases correspond respectively to the three symmetries SO(6), U(5), and SU(3) of the IBM approach. Obviously these extremes situations are ideal cases not met in realistic situations. Shape-phase transitional nuclei occur then between regions of these three limiting cases. It is well know that the GBH works better for regions that are far away from closed shells. Because in the general case there is no analytical solution, one needs then to solve numerically the Bohr Hamiltonian. Among the numerous methods we have chose the one of Libert (with its FORTRAN code) Ref. [24]. The calculations are done in two steps: (1) One builds the representative matrix of the Bohr Hamiltonian with the help of a suitable basis and then (2) One diagonalizes this Matrix. Beside the collective states obtained with this method it is also possible to deduce other observables such as electric or magnetic transitions probabilities, equilibrium shapes for ground state, etc...

III. THE MICROSCOPIC MODEL, SOME NUMERICAL DETAILS:

In this work, single-particles energies and wave functions are obtained by the diagonalization of the Schrödinger equation of the stationary states.

$$\hbar \phi_i(r) = \epsilon_i \phi_i(r)$$

$\epsilon_i$ and $\phi_i(r)$, are respectively, the eigenenergies and the eigenfunctions of the single-particle Hamiltonian $h$

$$h = -\frac{\hbar^2}{2m} \nabla M_{\text{eff}}(r) \nabla + V(r) - (\kappa / \hbar) (\nabla W_{\text{so}}(r) \times \mathbf{p}) \sigma + e \Phi_{\text{Coul}}(r)$$

This Hamiltonian contains four contributions. They are respectively: (1) the Kinetic energy operator, (2) the deformed central mean field, (3) the spin-orbit contribution, and (4) the Coulomb energy for the protons. The quantities $M_{\text{eff}}(r), V(r), W_{\text{so}}(r), \Phi_{\text{Coul}}(r)$ are respectively the effective mass field, the deformed central mean field, the deformed spin-orbit mean field and the Coulomb mean field ($\sigma$ denotes here the Pauli spin-matrices). For simplicity we have took $M(r) = 1$.

Single-particle Hamiltonian given by [3] has exactly the same structure as that obtained from the Hartree-Fock self-consistent method with an effective nucleon-nucleon interaction of the Skyrme III type. In our method we have simply replaced the self-consistent one body potentials $V(r), W(r)$ by phenomenological deformed mean fields of the
Woods-Saxon type. However for the protons the Coulomb potential has been approximated by the one of a continuous liquid deformed model with a sharp nucleus surface. For the Woods-Saxon potential the universal parameters’ of Ref. [27] have been used (see also Ref. [28]). This set of parameters claims to be able to reproduce the correct sequences of the single-particle levels and also the nuclear equilibrium deformations throughout the entire chart of nuclei [29, 30]. This set is the one of $^{118}$Xe, it is given in Table I.

Single-particle states in Eq. (2) are solved by the FORTRAN code of Ref. [25]. With these single-particle states we calculate the potential energy surfaces of the nucleus (deformation energy) by means of the macroscopic-microscopic method. The shell correction is calculated by a semiclassical approach of the Strutinsky method [31]. This means that we simply replace the Strutinsky level density by the semiclassical one. This allows us to avoid the well-known drawbacks (smoothing parameters) of this method. The pairing interaction is taken into account by the BCS approximation.

We give below some "technical" details of the calculations.

The deformation energy is defined as the liquid drop energy plus shell and pairing corrections:

$$E_{def}(N, Z, \beta, \gamma) = E_{LD}(N, Z, \beta, \gamma) + \delta E_{sc}(N, \beta, \gamma) + \delta E_{ac}(Z, \beta, \gamma) + \delta P(N, \beta, \gamma) + \delta P(Z, \beta, \gamma)$$

Where the liquid drop energy is given by:

$$E_{LD}(N, Z, \beta, \gamma) = \frac{3}{5} \frac{e^2 Z^2}{r_0 A^{1/3}} \left[ \frac{A}{2Z^2} \zeta \left[B_s(\gamma, \beta) - 1\right] + \left[B_c(\gamma, \beta) - 1\right] \right]$$

in which where $B_s$ and $B_c$ are the (normalized) surface and Coulomb contributions to the liquid drop. In the liquid drop model we have taken as in Ref. [32]: $r_0 \approx 1.275$ fm, and $\zeta = 52.8(1 - 2.84 I^2)$, $I = (N - Z)/(N + Z)$

The microscopic shell corrections $\delta E_{sc}$ are evaluated separately for neutrons and protons. They are defined as the difference between a sharp sum and a smoothed sum (between brackets) of the energy levels:

$$\delta E_{shell}(N or Z, \beta, \gamma) = 2 \sum \epsilon_k - 2 \left( \sum \epsilon_k \right)$$

with

$$\left( \sum \epsilon_k \right) = \int_{-\infty}^{\lambda_{sc}} \epsilon g_{sc}(\epsilon) d\epsilon \tag{7}$$

Here $g_{sc}$ is the semiclassical level density (which by definition does not contain shell effects ) and $\lambda_{sc}$ is the corresponding Fermi level which is fixed by a constraint on the particle-number. The factor 2 is due to the time-reversal symmetry. At last, it is worth to mention that the deformation dependence of the shell correction is contained through the eigenvalues $\epsilon_k$ which depend themselves on the nuclear quadrupole deformation $(\beta, \gamma)$.

The pairing correction $\delta P$ is evaluated (also separately for protons and neutrons) with the same method as in Ref. [33].

$$\delta P_{pairing}(N or Z, \beta, \gamma) = P - \overline{P} \tag{8}$$

where the pairing energy $P$ and the "average or smooth" pairing energy $\overline{P}$ are given by:

$$P = \sum_{k=1}^{N_p} 2\epsilon_k^2 - \frac{\Delta^2}{G} = \sum_{k=1}^{N_p/2} 2\epsilon_k, \quad \overline{P} = \frac{1}{2} g_{ac}(\lambda) \Delta^2 \tag{9}$$

TABLE I: Parameters of the Woods-Saxon potential.

| neutrons | | protons | |
|----------|----------|----------|----------|
| $V_0 = -45.99$ MeV | potential depth | $V_0 = -53.22$ MeV | |
| $a_V = 0.70$ fm | potential diffuseness | $a_V = 0.70$ fm | |
| $R_V = 6.61$ fm | potential radius | $R_V = 6.25$ fm | |
| $\kappa = 17.74$ MeV fm$^2$ | spin-orbit coupling | $\kappa = 21.13$ MeV fm$^2$ | |
| $a_{so} = 0.70$ fm | spin-orbit diffuseness | $a_{so} = 0.70$ fm | |
| $R_{so} = 6.42$ fm | spin-orbit radius | $R_{so} = 5.88$ fm | |
| | charge radius | $R_{ch} = 6.25$ fm | |
The number of levels used in calculations is defined in formula V3 of Ref. [33]. The microscopic moments of inertia and mass parameters are calculated in the usual cranking approximation of Inglis-Belyaev:

\[ \Theta_k = 2\hbar^2 \sum_{\nu, \mu} |\langle \nu | j_k | \mu \rangle|^2 \frac{(u_{\nu} v_{\mu} - u_{\mu} v_{\nu})^2}{E_\nu + E_\mu}, \quad k = 1, 2, 3 \]  \hspace{1cm} (10)

\[ D_{ij} = 2\hbar^2 \sum_{\nu, \mu} \langle \nu | \frac{\partial h}{\partial i} | \mu \rangle \langle \mu | \frac{\partial h}{\partial j} | \nu \rangle \frac{(u_{\nu} v_{\mu} + u_{\mu} v_{\nu})^2}{(E_\nu + E_\mu)^3}, \quad i, j = \beta \text{ or } \gamma \]  \hspace{1cm} (11)

Here \( i, j \) represent the quadrupole deformation parameters \( \beta \) or \( \gamma \), \( j_k \) is the single-particle angular momentum and \( h \) the single-particle Hamiltonian. The quantity \( E_\nu = \sqrt{(\epsilon_\nu - \lambda)^2 + \Delta^2} \) represents as usual the energy of the quasiparticle and \( u_\nu^2 = 1 - v_\nu^2 \) is related to the occupation probability of the level \( \nu \).

IV. RESULTS:

From numerous calculations based on microscopic evaluations of the inertial functions (i.e. with no free parameters in the GBH), it turns out that generally real difficulties are encountered to reproduce properly the experimental collective levels. Among these difficulties is the fact that the scales of theoretical collective spectra are generally too stretched compared to the experimental ones. "Fine structure" such as the order of the levels and their relative positions become then a challenge and it is not easy to correct these defects. This is because the seven functions of the GBH cannot be deduced directly from experiment and hence cannot be known without ambiguity. Moreover it often happens for the same model that good predictions in theoretical spectra are not "corroborated" by good probability transitions and vice-versa.

In the following our theoretical spectra will be compared to the ones deduced experimentally and compiled in the websites: http://www.nndc.bnl.gov/endsf.

Our main results can be summarized as follows:

The spectra obtained by our calculations are given in figures 1 and 2 at the left hand side for each isotope. The theoretical low energy levels are grouped in sets.

FIG. 1: Theoretical collective levels calculated by the General Bohr Hamiltonian with potential energy surface and inertial functions evaluated by means of microscopic method using the Woods-Saxon potential. We consider here only quadrupole collective level. The parity of the theoretical levels is therefore positive. This is the reason why it is simply omitted.
Nevertheless we obtain also bad results such as for the mean values of the ground states quadrupole deformation. Moreover as already noted the energy ratios given by our model in Fig.3 are quite close to the experimental ones. The calculated levels 2
whereas in Ref. [16] it is corrected by reducing artificially the pairing strengths by 20%. The second satisfaction is of Ref. [15] the stretching of the collective spectra is "cured" by introducing the pairing vibrations in the calculations Saxon mean field which gives the right values for the mass parameters. In earlier similar works, for example the one words the usual defect of the stretching [14] of the spectra is not present. This seems essentially due to the Woods-Saxon mean field which gives the right values for the mass parameters can be considered as constant.

Above the doublets we find either a set of the type (2+
energy ratios (ii) Moreover the mass parameters
B
ββ
are for the most nuclei very close to the experimental ones. All other nuclei are characterized by doublets (4+, 2+).

This suggests that these nuclei have a spectrum structure close to the one of the γ unstable nuclei of Wilets-Jean model which predicts the doublet (4+, 2+).

We recall that the Wilets-Jean model is essentially based on the hypothesis that the potential energy does not depend on the axial asymmetry γ [35], i.e. \( \partial U_{\text{col}}(\beta, \gamma) / \partial \gamma = 0 \) with a strong minimum out of the spherical shape (i.e. the minimum occurs for \( \beta \neq 0 \)). These nuclei are aften called as to be γ−soft. In this respect, it is possible to consider the harmonic vibrator as a particular case of the Wilets-Jean model. In effect, the Wilets-Jean model is defined by the condition \( \partial U_{\text{col}}(\beta, \gamma) / \partial \gamma = 0 \) which is filled by the harmonic vibrator. The only difference comes from the fact that the minimum of the collective potential energy occurs for the spherical shape whereas in the W-J model it lies elsewhere. Consequently, it is then not surpising that among them two are of vibrational type.

It is easy to explain why our theoretical values are close to the ones of the anharmonic vibrator:
(i) The potential energy depends very little on the axial asymmetry parameter γ (as for Wilets-Jean model)
(ii) The deformation energy (defined as the difference between the energy for the spherical shape and the one obtained for the equilibrium deformation) is too weak. In other words these nuclei are theoretically too "soft" in the β degree of freedom and the well is insufficiently pronounced for \( \beta \neq 0 \) to obtain Wilets-Jean potential type.
(iii) Moreover the mass parameters \( B_\beta, B_\gamma, B_{\gamma\gamma} \) vary very little in the vicinity of the minimum. Therefore as in the original Bohr model the mass parameters can be considered as constant.

Above the doublets we find either a set of the type (2+, 3+, 4+, 6+) or of the type (0+, 2+, 3+, 4+, 6+). The experimental energy ratios \( E(4^+_1)/E(2^+_1) \) lie between the the γ−soft and the vibrational limits in Fig.[3] but are much more closer to the γ−soft limit especially for the last isotopes. The theoretical values are not so far away from the experimental ones but their behaviours as a function of A seem to be opposite from each other.

The first satisfaction of these calculations is the correct scale of the spectra without any kind of correction. In other words the usual defect of the stretching of the spectra is not present. This seems essentially due to the Woods-Saxon mean field which gives the right values for the mass parameters. In earlier similar works, for example the one of Ref.[15] the stretching of the collective spectra is "cured" by introducing the pairing vibrations in the calculations whereas in Ref. [16] it is corrected by reducing artificially the pairing strengths by 20%. The second satisfaction is the calculated levels \( 2^+_1 \) and the doublets \( (4^+_1, 2^+_1) \) which are for the most nuclei very close to the experimental ones. Moreover as already noted the energy ratios given by our model in Fig.[3] are quite close to the experimental ones. Nevertheless we obtain also bad results such as for the mean values of the ground states quadrupole deformation \( \langle \beta \rangle \) in Fig.[4] The experimental values are deduced from transitions probabilities \( B(E2; 0^+ \rightarrow 2^+) \) from the website.

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**FIG. 2: Continuation of Fig. 1**

They are characterized by a structure which is very close to that of the five dimensional (anharmonic) vibrator. The triplets \( (0^+, 2^+, 4^+) \) and the quintuplets \( (0^+, 2^+, 3^+, 4^+, 6^+) \) are as a rule, present for all the isotopes, \( ^{112−126}Xe \). However, experimental data given at the right hand side for each isotope show that only two nuclei belong to this type, namely \( ^{118}Xe \) and \( ^{120}Xe \) which are well described here. All other nuclei are characterized by doublets \( (4^+, 2^+) \).

As for Wilets-Jean model the mass parameters can be considered as constant. The potential energy depends very little on the axial assymmetry parameter \( \gamma \) [35], i.e. \( \partial U_{\text{col}}(\beta, \gamma) / \partial \gamma = 0 \) with a strong minimum out of the spherical shape (i.e. the minimum occurs for \( \beta \neq 0 \)). These nuclei are aften called as to be γ−soft. In this respect, it is possible to consider the harmonic vibrator as a particular case of the Wilets-Jean model. In effect, the Wilets-Jean model is defined by the condition \( \partial U_{\text{col}}(\beta, \gamma) / \partial \gamma = 0 \) which is filled by the harmonic vibrator. The only difference comes from the fact that the minimum of the collective potential energy occurs for the spherical shape whereas in the W-J model it lies elsewhere. Consequently, it is then not surpising that among them two are of vibrational type.

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FIG. 3: Energy ratio $E(4^+_{1^+})/E(2^+_{1^+})$ for the family of isotopes $^{112-126}$Xe.

http://www.nndc.bnl.gov/be2 whereas the deformations given by the FORTRAN code come from the collective wave function ($B(E2; 0^+ \rightarrow 2^+)$ values are not calculated by the present version of the code).

FIG. 4: Root mean Square value $\sqrt{\langle \beta^2 \rangle}$ of the quadrupole deformation in the ground state as function of the mass number for the Xenon isotopes.

V. CONCLUSION

Microscopic calculations based on the Woods-Saxon mean field were performed to find the potential energy and the six inertial functions entering into the collective Bohr hamiltonian. We have considered the light and medium Xenon isotopes of the region $112 < A < 126$. Then, the Bohr hamiltonian has been diagonalized without any fitting of parameters. The resulting spectra were found to be quite close to the experimental ones. Moreover the values of the mass parameters seemed to be correct in magnitude giving a good scaling in the collective spectra for this region. Most of theoretical collective levels $E(2^+_{1^+})$ were found to be in good agreement with the experimental ones. The theoretical energy ratios $E(4^+_{1^+})/E(2^+_{1^+})$ were also fairly well. However, the major difference comes from the fact that our spectra belong to the (anharmonic) vibrator type whereas most of experimental spectra exhibit doublets of the Wilets-Jean model. Both alike are of the same type ($\gamma-$soft), however contrarily to the Wilets-Jean model, our collective potential energy does not posses a sharp minimum for a deformed shape ($\beta \neq 0$). In other words the shell correction is not sufficiently strong to modify significantly the potential energy of the liquid drop model. Consequently some further studies seem to be necessary in order to correct this defect.
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