Studiu-raport de cercetare nr. 3 (final)

Proiectului de cercetare: *"Aplicaţii ale analizei matematice în teoria numerelor, optimizare, ecuaţii diferenţiale, alte domenii de cercetare matematică sau multidisciplinară"*

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Obiectul raportului: Raportul are ca obiect activitatea de cercetare desfăşurată pentru îndeplinirea celor două obiective ale sale:

1. *"Descrierea semiclasică a geometriei chirale a sistemelor cu dinamică rotaţională complexă"*
2. *"Descrierea unei tranziţii de fază de ordinul unu în forma nucleelor γ-instabile cu ajutorul unui potenţial sextic."*

Ataşat acestui raport este forma finală a lucrării ce prezintă rezultatele obţinute prin îndeplinirea celor două obiective. În cele ce urmează voi prezenta pe scurt concluziile reeşite din acest studiu ce fac obiectul acestui raport de cercetare final.

Diferenţa esenţială dintre cele două probleme studiate în cadrul acestui proiect de cercetare este prezenţa unei simetrii adiţionale în cazul unidimensional asociat primei probleme. Într-adevăr, problema unidimensională este invariantă la transformarea de paritate. Această simetrie adiţională întroduce un nou număr cuantic corespunzător parităţii funcţiei de undă, astfel încât numărul stărilor distincte este dublat. Această multiplicare a stărilor proprii se întâmplă deasemenea şi în cazul potenţialelor cu două gropi asimetrice. Această caracteristică poate fi observată mai bine atunci când bariera ce separă minimile simetrice corespunzătoare variabilei pozitive şi respectiv negative este crescută suficient de mult ca să blocheze complet tunelarea dintre ele. Energia totală asociată acestui caz la limită poate fi considerată ca fiind corespunzătoare unei probleme simple pentru o singură groapă dar cu degenerare dublă a spectrului. Mai mult de atât, funcţia de undă totală corespunzătoare la cele două nivele degenerate poate fi exprimată ca o combinaţie liniară simetrică şi respectiv asimetrică a funcţiilor de undă pentru vibraţia separată în fiecare dintre cele două gropi de potenţial.

În probleme radiale pentru potenţiale cu două gropi nu există însă nici o simetrie în plus. Chiar dacă se poate construi oricând un potenţial radial cu două gropi simetrice faţă de bariera separatoare, funcţiile de undă asociate nu vor avea această simetrie. Astfel, spectrul total în astfel de cazuri nu mai este dublat. Deasemenea, cum nu mai este nici o simetrie asociată, stările corespunzătoare nu mai pot fi interpretate ca superpoziţii a două stări *"clasice"* de nedeosebit localizate în fiecare din cele două gropi ale potenţialului.

Când bariera unui potenţial radial cu două gropi este foarte înaltă şi cele două gropi sunt separate suficient de mult pentru a nu interacţiona prin tunelare, se constată că starea fundamentală este deja localizată în una dintre gropi. Mai concret, starea fundamentală preferă în acest caz groapa mai depărtată. Un alt aspect interesant se referă la faptul că în aceleaşi condiţii ale unei bariere separatoare foarte înalte, prima stare excitată îşi pierde complet caracterul vibraţional, adică funcţia sa de undă nu mai posedă un nod. Deasemenea starea excitată devine şi ea localizată, doar că în groapa cea mai apropiată de origine.

În concluzie, pentru bariere separatoare foarte înalte, starea fundamentală în cazul unidimensional al potenţialului cu două gropi simetrice este dublu degenerată şi are aceiaşi distribuţie de probabilitate de localizare în ambele gropi. Unica distincţie dintre cele două stări este dată de paritatea acestora la schimbarea semnului variabilei. Contrar acestei comportări, starea fundamentală şi prima stare excitată au energii diferite în cazul problemei radiale pentru un potenţial cu două minime. Fiecare din aceste stări sunt şi localizate doar în unul din cele două gropi de potenţial.

Când bariera separatoare este micşorată astfel încât să permită tunelarea cuantică prin ea dintre cele două gropi de potenţial, degenerarea stărilor din cazul unidimensional simetric este ridicată. Cele două stări îşi păstrează încă proprietăţile de paritate şi distribuţia de probabilitate de localizare în ambele gropi, totuşi ne mai fiind egal distribuită între cele două gropi. Pe măsură ce bariera scade şi mai mult, spectrul energetic total devine regular şi similar celui associat unei singure gropi de potenţial. Permiţând acum tunelarea în cazul problemei radiale cu două gropi, conduce la redistribuirea probabilităţii de localizare a fiecărei stări în ambele gropi de potenţial. Startul acestui fenomen marchează şi apariţia nodului în prima stare excitată, ceea ce îi conferă un caracter vibraţional. Pentru anumite forme ale potenţialului cu două gropi, distribuţia de probabilitate de localizare pentru starea fundamentală poate să prezinte chiar şi o structură cu două vârfuri. Această situaţie nu este condiţionată de degenerarea minimelor celor două gropi de potenţial.

În final, studiul sistemelor fizice cu ajutorul potenţialelor cu două gropi dezvălue aspecte analitice noi. Mai mult de atât, datorită faptului că fiecare problemă tratată în acest studiu se referă la fenomene fizice reale, efectele de mecanică cuantică reeşite capătă şi o interpretare fizică.

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Applications of double well potentials in the collective nuclear motion

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Abstract

The recent applications of double well potentials in the description of shape coexistence phenomena and chiral symmetry breaking in nuclear physics is discussed with an emphasis on the analytical properties of the corresponding wave functions. By means of the density of probability distribution, the effect of the quantum tunneling on the composition of the wave functions is dully investigated. The results are used to identify the distinctive features between the one-dimensional and central multidimensional problems.

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keywords: Schrödinger equation, Double well potentials, Quantum tunneling, Nuclear collective motion, Triaxial rigid rotor, Bohr Hamiltonian.

1 Introduction

The numerical solution of the Schrödinger equation for a double-well potential is thoroughly studied in the one-dimensional case. This is due to its importance for the understanding of the unconventional nature of the quantum mechanics. More precisely, its solution is a perfect example of superposition between two "*classical*" states associated to the system being

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in one or the other potential well. The one-dimensional double well potential, and especially its symmetric variety is a constant presence throughout all fields of physics, but has a particular importance in the quantum field theory and molecular physics. In the first case, it is closely related to the instanton theory and is used to investigate gauge fields with degenerate vacua [1]. While in molecular physics it is extensively used to study the vibration of non-planar molecules [2]. The most used example in this case [3, 4] is the ammonia molecule where the Nitrogen atom can pass through the plan of the three Hydrogen atoms with minimal energy expense. The two spatial configurations are then modeled as degenerated minima of a symmetric one-dimensional potential. In nuclear physics, geometrical three body configurations of two nucleons and a collective core exhibit similar symmetry properties. In particular, the alignment of the ellipsoidal trajectories of the valence nucleons to the intrinsic reference frame of the core deformation such that a three-dimensional geometry is obtained lead to two "*classical*" states where the system is right or left-handed [5]. Such a system is said to have a chiral symmetry. The superposition of these pure states can be understood through a one-dimensional Hamiltonian with a double well potential for a suitably chosen chiral variable. Such a Hamiltonian was for the first time constructed in Ref.[6] as a sum of a kinetic operator with a coordinate dependent mass term and a chiral potential which are both microscopically determined through distinct ways. A qualitatively similar result can be obtained by treating semiclassically a displaced rotor Hamiltonian which have the advantage of analytical formulas as well as of the fact that both mass term and the chiral potential are obtained in a consistent way from a coherent theory [7, 8]. Regarding the use of double well potentials in nuclear collective motion, one could also mention the Interacting Boson Model description of prolate-oblate shape coexistence [9] and the boson expansion approach on the wobbling excitations [10, 11].

There is however extremely little investigation into central problems with double well potentials. The time-independent Schrödinger equation in the multi-dimensional case becomes a partial differential equation and the nature of the barrier for motion along different degrees of freedom is different. Moreover, the symmetry properties of the one-dimensional problem are no longer applicable to the hyper-radial equation. In nuclear physics, double well radial potentials are often encountered in various types of fission processes [12]. With the advent of computational prowess, the microscopically determined multiple minima potential energy surfaces in shape variables can be used as numerical potentials for collective excitations within the five-dimensional space of shape variables defining the dynamical deformation of

a nucleus [13]. Although such approaches make the long sought connection between microscopic and collective degrees of freedom, it lacks in physical transparency leading thus to misinterpretations of various geometric characteristics of the nuclear shape because the microscopic input is fixed to reproduce only intrinsic bulk properties. Traditionally, the collective aspects of the nuclear shape are described through algebraic and geometric models which provide an intuitive picture through the analytical and closed form of the potential energy. Despite the fact that algebraic model calculations with multiple minima potentials are analytically complex and still computationally demanding, the interest in them is increasing due to their connection to the very active topic of nuclear shape coexistence. A recent contribution in this sense was made in Refs.[14, 15, 16], where a computationally feasible approach to solve Bohr Hamiltonian problems with double minima collective potentials was proposed.

In this study, one will present some analytical aspects of the one-dimensional and five-dimensional double well problems used to describe the chiral geometry found in some odd mass nuclei and respectively the phenomenon of shape coexistence in even-even nuclei. Due to relatively uncharted territory of the central double well potentials, the discussion will be focused on the comparison between the two pictures.

2 One-dimensional double well chiral vibration

The chiral geometry in nuclear systems comes down to a spacial configuration where a triaxial collective core tends to rotate around the axis with the largest moment of inertia while sets of particles and holes follow ellipsoidal orbits around mutually perpendicular axes [17]. The system of three mutually perpendicular angular momenta can compose the same total angular momentum vector by means of a right-handed and respectively a left-handed trihedral arrangement. The relevant Hamiltonian associated to two single-particle spins rigidly aligned along the intrinsic axes 1 and 2 can be written as [8]

$$H_{chiral} = A_1\hat{I}_1^2 + A_2\hat{I}_2^2 + A_3\hat{I}_3^2 - 2A_1 j\hat{I}_1 - 2A_2 j'\hat{I}_2, \tag{1}$$

where A_k are inertial parameters along the principal axes of the intrinsic frame of reference while I_k are the operators of the total angular momentum projections on the same axes.

The quantum Hamiltonian (1) is studied then within a time dependent

variational principle with the help of the variational state

$$\begin{aligned} |\psi(x,\phi)\rangle &= \sum_{K=-I}^{I} \frac{1}{(2I)^I}\sqrt{\frac{(2I)!}{(I-K)!(I+K)!}} \\ &\times (I+x)^{\frac{I-K}{2}}(I-x)^{\frac{I+K}{2}} e^{i\varphi(I+K)}|IMK\rangle, \end{aligned} \tag{2}$$

which is actually a coherent state for the $SU(2)$ algebra of the angular momentum operators parametrized by the azimuth angle φ defining the direction of the total angular momentum vector in the plane of the two single particle spins and the so called chiral variable x which is just the angular momentum projection on the third intrinsic axis. By solving the variational principle, one obtains a classical energy function:

$$\begin{aligned} \mathcal{H}(x,\varphi) &= \frac{I}{2}(A_1+A_2)+A_3I^2+\frac{(2I-1)(I^2-x^2)}{2I} \\ &\times (A_1\cos^2\varphi + A_2\sin^2\varphi - A_3) - \\ &2A_1 j\sqrt{I^2-x^2}\cos\varphi - 2A_2 j'\sqrt{I^2-x^2}\sin\varphi, \end{aligned} \tag{3}$$

and a set of equations of motion for x and φ. The later have a Hamilton canonical form and therefore identify the two parameters as classical canonical variables, with the chiral variable playing the role of a generalized momentum. After a certain critical value of the total angular momentum I and when special conditions defined by the inertial parameters are satisfied, the classical energy function exhibits two minima in respect to the chiral variable x. The two stationary points correspond to the geometrical configurations with different handedness or chirality. In order to extract the quantum energy states corresponding to the two chiral partners, one first need to quantize the classical energy function. This is done by expanding it around the corresponding minimum points in φ for fixed values of x:

$$\tilde{\mathcal{H}}(x,\varphi) \approx \mathcal{H}(x,\varphi_0(x)) + \frac{1}{2}\left(\frac{\partial^2\mathcal{H}}{\partial\varphi^2}\right)_{\varphi_0(x)} [\varphi-\varphi_0(x)]^2 . \tag{4}$$

$\varphi_0(x)$ is the value which minimizes the energy function for a fixed x and is determined by solving the following equation

$$\begin{aligned} &(2I-1)\sqrt{I^2-x^2}(A_2-A_1)\cos\varphi_0(x)\sin\varphi_0(x) \\ &= 2I\left[A_2 j'\cos\varphi_0(x) - A_1 j\sin\varphi_0(x)\right]. \end{aligned} \tag{5}$$

It has a simple analytical solution only for the case when $A_1 = A_2$. Substituting now $\varphi-\varphi_0(x)$ with $i\frac{d}{dx}$ in the properly symmetrized Eq.(4) one

arrives at a quantum Hamiltonian expressed as the differential operator

$$\hat{H}_c = -\frac{1}{2}\frac{1}{\sqrt{B(x)}}\frac{d}{dx}\frac{1}{\sqrt{B(x)}}\frac{d}{dx} + V(x), \tag{6}$$

where

$$B(x) = \left[\frac{\partial^2 \mathcal{H}(x,\varphi)}{\partial \varphi^2}\right]^{-1}_{\varphi_0(x)}. \tag{7}$$

plays the role of an one-dimensional mass which depends on x, while the chiral potential is expressed as:

$$V(x) = \mathcal{H}(x,\varphi_0(x)) + \frac{B''(x)}{8\left[B(x)\right]^2} - \frac{9\left[B'(x)\right]^2}{32\left[B(x)\right]^3}. \tag{8}$$

For the generality of the formalism, one presents here the full analytical expression for the mass term

$$\begin{aligned}[B(x)]^{-1} &= \frac{\sqrt{I^2-x^2}}{I}\Big[(2I-1)\sqrt{(I^2-x^2)}(A_2-A_1)\cos\left(2\varphi_0(x)\right) \\ &\quad +2A_1 jI\cos\left(\varphi_0(x)\right) + 2A_2 j' I\sin\left(\varphi_0(x)\right)\Big], \end{aligned}\tag{9}$$

which is then used to define the chiral potential. In the special case when $A_1 = A_2 = A$, the azimuth angle which minimizes the classical energy, becomes independent of x and has the constant value of $\pi/4$. These conditions lead to a very simple expression for the mass term:

$$B(x) = \frac{1}{\sqrt{2}A\sqrt{I^2-x^2}(j+j')}. \tag{10}$$

With this, the potential can be easily written explicitly as a function of the chiral variable. Here one will give the expression for the case when $j = j' = 11/2$ which is more studied from the experimental point of view:

$$\begin{aligned}V(x) &= -\frac{11\sqrt{2}\left[32I^4 - 4I^2\left(16x^2+1\right) + 32x^4 + x^2\right]}{32\left[(I-x)(I+x)\right]^{3/2}} \\ &\quad +\frac{3(1-2I)x^2}{16I} + \frac{2I(8I+5)}{16}. \end{aligned}\tag{11}$$

It can be easily checked that both mass function and the potential are invariant under the parity transformation $x \to -x$. Therefore the potential is symmetrical and has two degenerated minima. Additionally, the exact eigenfunctions satisfy the Dirichlet boundary condition at $x = I$ and $x = -I$.

The formalism is easily transposable to other single-particle spin combinations of j and j'. By numerical calculations one ascertained that for smaller and equal single-particle spins $j = j' = 9/2$, the potential is higher in energy with sharper minima delimited by a higher barrier at $x = 0$. The same behaviour is found when only the total angular momentum value is raised. The separating barrier is actually a parabola. This can also be seen from the analytical expression (11), where the quadratic term is dominant for small x.

Due to the symmetry of the problem, the solutions can be separated by the parity. As the corresponding eigenvalue problem cannot be solved exactly, this property comes in handy when considering a diagonalization procedure. Indeed, one can use different basis states with certain parity properties in order to reduce the diagonalization dimension by half. One of the most often employed diagonalization basis states for such symmetrical problems are the particle in the box eigenstates or simply the trigonometric basis [18, 19]. Assigning now for each parity the basis states:

$$g_n^1(x) = \frac{1}{\sqrt{I}} \cos\left[\frac{(2n-1)\pi x}{2I}\right],\ n = 1, 2, ..., \tag{12}$$

$$g_n^{-1}(x) = \frac{1}{\sqrt{I}} \sin\left[\frac{2n\pi x}{2I}\right],\ n = 1, 2, ... \tag{13}$$

where 1 denotes even parity, while -1 the odd parity states, the eigenvalues and the eigenfunctions are then easily obtained through a diagonalization procedure using a basis dimension which achieves a desirable convergence of the diagonalization results. For the purpose of the numerical applications made on the chiral bands of ^{134}Pr nucleus, the truncation of the basis was set to 50. The states of the two chiral bands are defined as the first two eigenvalues of the chiral potential for a given total angular momentum value. The first chiral state is found to be symmetrical, while the second one which has a higher energy is antisymmetrical. The splitting between the two chiral eigenvalues depends on the amount of tunneling allowed by the barrier between the two symmetrical potential wells. As the barrier increases by considering higher angular momentum values, the two potential wells are no longer interacting, and the spectra associated to the two minima become degenerated.

3 Sextic potential with double minima for the five-dimensional Bohr Hamiltonian

The nuclear collective motion associated to quadrupole degrees of freedom is traditionally studied by means of the Bohr Hamiltonian [20]:

$$\begin{aligned} H &= -\frac{\hbar^2}{2B}\left[\frac{1}{\beta^4}\frac{\partial}{\partial\beta}\beta^4\frac{\partial}{\partial\beta}+\frac{1}{\beta^2\sin 3\gamma}\frac{\partial}{\partial\gamma}\sin 3\gamma\frac{\partial}{\partial\gamma}\right. \\ &\quad \left.-\frac{1}{4\beta^2}\sum_{k=1}^{3}\frac{Q_k^2}{\sin^2\left(\gamma-\frac{2}{3}\pi k\right)}\right]+V(\beta,\gamma). \end{aligned} \tag{14}$$

B is the mass parameter which in general collective model is actually included in a mass bi-tensor in five dimensional space of the shape and angle variables. $Q_k(k=1,2,3)$ designate the three projections of the angular momentum on the principal axes of the intrinsic frame of reference defined by the principal axes of the spheroid representing the deformed nuclear shape. β shape variable represents the deviation from the spherical nuclear shape, while the γ variable is associated to the deviations from axiallity in the presence of a non-vanishing β deformation. Finally, the Euler angles expressing the angular momentum operators are associated to the rotational motion of the nucleus. There are experimental evidences of a possible adiabatic separation of β shape fluctuations and coupled γ-angular excitations. This situation can be modeled by assuming a separable potential of the form $V(\beta,\gamma)=[v(\beta)+u(\gamma)]\hbar^2/2B$, as in case of the well known X(5) model [21]. With a total wave function factorized as $\Psi(\beta,\gamma,\Omega)=f(\beta)F(\Omega,\gamma)$ one separates the Eq.(14) in two second order differential equations: one corresponding to the β shape variable, and another one to the γ-angular degrees of freedom. In the case of mostly prolate nuclear shapes, when the γ potential is very sharp and centered around $\gamma=0$, the rotational term from (14) can be approximated as

$$\sum_{k=1}^{3}\frac{Q_k^2}{\sin^2\left(\gamma-\frac{2}{3}\pi k\right)}\approx\frac{4}{3}\mathbf{Q}^2+Q_3^2\left(\frac{1}{\sin^2\gamma}-\frac{4}{3}\right). \tag{15}$$

$\mathbf{Q}$ is the total angular momentum vector operator whose eigenfunctions, which are common also to the operator of the third component of angular momentum, are the Wigner rotational matrices D^L_{MK} of total angular momentum L and its projections M and K on the body-fixed third axis and laboratory-fixed z axis, respectively. This approximation allows a second

separation of variables, more precisely of γ shape variable from the rotational degrees of freedom. Now, averaging the separated β equation on the rotational matrices, one obtains the following differential equation:

$$\left[-\frac{1}{\beta^4}\frac{\partial}{\partial\beta}\beta^4\frac{\partial}{\partial\beta}+\frac{L(L+1)}{3\beta^2}+v(\beta)\right]\Psi(\beta)=\epsilon^\beta\Psi(\beta), \tag{16}$$

which describes the rotation-vibration states with the projection quantum number $K=0$ and positive parity, restricting thus the spectrum only to even angular momentum states. The energy of the above equation is scaled as in the case of the potential, that is $\epsilon^\beta=2BE/\hbar^2$.

Due to the separation of the β degree of freedom, and the symmetry restrictions on the collective potential, the associated β potential must be a polynomial in β^2. The simplest potential which can achieve simultaneous spherical and deformed minima needed for the description of shape coexistence is the sextic potential:

$$v(\beta)=a\beta^2+b\beta^4+c\beta^6. \tag{17}$$

It can be easily checked that Eq.(16) for the above potential have a scaling property which lead to the equivalence:

$$\epsilon^\beta(a,b,c)=a^{1/2}\epsilon^\beta(1,ba^{-3/2},ca^{-2}). \tag{18}$$

Thus, solving only the eigenvalue equation for potentials:

$$v(\beta)=\beta^2+\mu\beta^4+\nu\beta^6, \tag{19}$$

is enough to determine the unique energy spectra up to a scale factor. This potential has two minima at

$$\beta_{min}=\begin{cases}0,\\ \sqrt{\frac{\sqrt{\mu^2-3\nu}-\mu}{3\nu}},\end{cases} \tag{20}$$

only if $\mu<0$ and $\nu>0$. Imposing additional restrictions on the potential consistent with the desired phenomenological needs, the potential and consequently the entire model will reduce to a single free parameter. For example in Refs.[22, 23, 24], the sextic potential was restricted to its quasi-exactly solvable instance, while in Refs.[14, 15] it was restricted to have two degenerated minima. In the later case, there was expected to find a splitting of the density probability for the ground state which would have been a clear indication of shape coexistence. The results, however revealed only

hints of fragmentation in the density probability of the ground state. The clearer indications of some kind of shape coexistence were observed in the β excited state. The reason for this hindering of the shape coexistence signatures resides in the fact that there is an additional centrifugal contribution coming from the multidimensional kinetic term of the Bohr Hamiltonian which raises the spherical minimum such that its effect is substantially subsided. This can be seen by changing the function as $\psi(\beta) = \Psi(\beta)/\beta^2$. With this change of function one can express the differential equation (16) in a one-dimensional Schrödinger form

$$\left[-\frac{\partial^2}{\partial\beta^2} + v_{eff}(\beta)\right]\psi(\beta) = \epsilon^{\beta}\psi(\beta), \tag{21}$$

for an effective potential

$$v^{L}_{eff}(\beta) = \frac{L(L+1)+6}{3\beta^2} + \beta^2 + \mu\beta^4 + \nu\beta^6. \tag{22}$$

As can be seen, even for the $L = 0$ states, the aforemention centrifugal contribution is non-vanishing and has the effect of raising and displacing the spherical minimum of the original potential $v(\beta)$. Therefore, although the original potential exhibit two minima, for certain values of parameters μ and ν the spherical minimum of the ground state effective potential can completely vanish. This problem was discussed in Ref.[16], where instead of employing two degenerated minima for the original potential $v(\beta)$, the same property is used on the effective potential in the ground state band. Although such a condition also renders the model to a single free parameter, the minimum condition for $v^{0}_{eff}(\beta)$ is a quartic equation in β^2 and therefore there is no analytical relationship between parameters μ and ν which realizes the mentioned conditions. Nevertheless, numerical calculations are possible and were carried out for few representative cases in order to ascertain the effect of the height and width of the barrier on the energy spectrum and on the probability distribution of the low lying states [16].

Solving the Schrödinger equation for multiple wells is not a trivial task, and is more complex for the multi-dimensional case with central symmetry. A highly effective procedure for solving such problems can be found in Refs.[25, 26, 27]. By adapting this prescription to the present case and particular numerical applications, the energies and the wave functions of (21) with effective ground state potentials having degenerated minima are determined through a diagonalization procedure using the basis states

$$\tilde{\Psi}_{\nu n}(\beta) = \frac{\sqrt{2}\beta^{-\frac{3}{2}} J_{\nu}(\alpha_n\beta/\beta_W)}{\beta_W J_{\nu+1}(\alpha_n)}. \tag{23}$$

Here J_ν are Bessel functions of the first kind with

$$\nu = \sqrt{\frac{9}{4} + \frac{L(L+1)}{3}}, \tag{24}$$

while $\alpha_n = \beta_W \lambda$ are their associated zeros indexed by the order $n = 1, 2, 3...$ and defined by the boundary conditions for a suitably chosen limiting value β_W which encompass the relevant part of the potential $v(\beta)$ [27]. The boundary value β_W is determined such that by increasing it, all considered energy states for a given dimension of the diagonalization basis would change no more than a preset precision [14]. Within the set of orthogonal functions (23), the Hamiltonian matrix to be diagonalized is

$$H_{nm} = \left(\frac{\alpha_n}{y_W}\right)^2 \delta_{nm} + \frac{2\sum_{i=1}^{3} v_i \left(y_W\right)^{2i} I_{nm}^{(\nu,i)}}{q^2 J_{\nu+1}(\alpha_n) J_{\nu+1}(\alpha_m)}, \tag{25}$$

where $v_1 == 1$, $v_2 = \mu$ and $v_3 = \nu$. The integrals

$$I_{nm}^{(\nu,i)} = \int_0^1 x^{2i+1} J_\nu(\alpha_n x) J_\nu(\alpha_m x) dx, \; x = \beta/\beta_W. \tag{26}$$

are numerically calculated using some recurrence relations [26, 27] which considerably optimize the procedure. The set of final eigenvalues for certain values of μ and ν which assure degenerate minima for the ground state effective potential and implicitly a fixed angular momentum L belong to different β vibrational bands. The ground band states are obviously identified with the lowest eigenvalues and so on. The eigenvector components found through the diagonalization procedure represent the coefficients of the basis expansion

$$\Psi_{Lk}(\beta) = \sum_{n}^{n_{max}} A_n^k \tilde{\Psi}_{\nu n}(\beta), \tag{27}$$

where k denotes the order of the solution and n_{max} is the truncated dimension of the diagonalization basis. This output is needed for the calculus of the electromagnetic transitions and other relevant observables such as averages and moments.

For the numerical calculation made so far in Refs.[14, 15, 16], one considered a basis with $n_{max} = 20$ states and an end precision for the diagonalization convergence as the boundary β_W is varied set to 10^{-7} units of the absolute energy.

The restriction to have degenerate minima in the ground state effective potential makes the barrier to increase in height and in thickness as the

relationship between μ and ν is changed. The numerical results in this case supports the conclusions made regarding the high barrier case, that is the complete separation of the ground band and excited band states, whose associated probability distribution have both single peak profiles localized in the deformed and respectively near-spherical potential wells. Decreasing the height and the thickness of the barrier, tunneling between the two deformation configurations becomes possible. Thus, the probability distribution of the ground state starts to spill into the first less deformed potential well, exhibiting at some point a double peak structure. The same happens with the probability distribution of the first β excited state, which through the same process recovers its usual role of an one phonon vibrational mode, with the two peaks representing the turning points of the classical vibration around the ground state average deformation. The vibrational nature of the first β excited state is also supported by the presence of a node in its wave function.

4 Discussion and concluding remarks

The major difference between the two problems presented above is the presence of an additional symmetry in the one-dimensional case. Indeed, the one-dimensional problem is invariant under the parity transformation. This additional symmetry introduces a new quantum number related to the parity of the wave function, such that the number of states is doubled up. The doubling of eigenstates happens also in the case of asymmetric double well problems. For the symmetrical problem, this feature can be observed when the barrier between the positive and negative variable minima of the potential is increased sufficiently to block any tunneling through it. The total energy spectrum associated to this limiting case can be regarded as corresponding to the simple one well problem but with double degeneracy of the spectrum [28]. Additionally, the wave functions corresponding to a doubly degenerated energy level can be expressed as symmetric and antisymmetric linear combinations of wave functions for vibration about each potential minimum [29].

In the radial type double well problem, there is no additional symmetry. Indeed, although one can always construct a double well radial potential with a symmetrical shape in respect to its barrier, the associated wave functions would not have this symmetry. Therefore, the total spectrum in such problems is not doubled. Moreover, as there is no symmetry regarding the two potential minima, the corresponding states cannot be interpreted as a

superposition of two "*classical*" undistinguishable states localized in each of the potential wells. Thus, when the barrier is very high and the two potential wells are sufficiently separated, the ground state is already localized in one of the potential minima. More precisely, it seems that in radial problems, the ground state prefer the potential well with its minimum point positioned at the highest value. It is interesting to find that for a very high separating barrier, the first excited state loses its vibrational nature, *i.e.* it no longer have a node. Moreover it is localized in the potential well with the minimum at the lowest value of the variable.

In conclusion, for very high separating barriers, the ground state and first excited state in one-dimensional symmetric double well problems are degenerated and have the same probability distribution with identical peaks in both potential wells. The only distinction is that the ground state wave function is symmetric, while the first excited state is anti-symmetric. In contradistinction, the radial problem for a double well potential provide very different energy levels for the ground and the first excited non-rotational states whose corresponding probability density distributions are single peaks localized in the second and respectively first potential well.

When the separating barrier is decreased such that to allow quantum tunneling through it between the two potential wells, the degeneration of states from the symmetrical one-dimensional case is lifted. The two states preserve their parity signature and their double peak probability distribution. As the barrier become smaller and smaller, the full energy spectrum becomes regular and similar to a single well potential problem. Allowing tunneling in the radial double well case, allows a gradual redistribution of the probability distribution for each state in both potential wells. This also marks the apparition of a node in the first excited state, fact which confers it a vibrational-like nature. For specific shapes of the radial double well potential, the probability distribution for the ground state can present a double peak structure which however is not conditioned by the degeneracy of the two potential minima.

In summary, the study of physical systems with the help of double well potentials reveals also some analytical aspects never discussed before. Moreover, given the fact that each problem corresponds to real physical phenomena, the encountered quantum mechanical effects acquire some physical interpretation.

References

[1] A.M. Polyakov. Quark confinement and topology of gauge theories. *Nucl. Phys. B* 120:429-458, 1977.

[2] G. Herzberg. *Molecular spectra and molecular structure. Electronic spectra and electronic structure of polyatomic molecules* Vol. II, Krieger, Malabar, FL, 1991.

[3] M.F. Manning. Energy levels of a symmetrical double minima problem with applications to the NH_3 and ND_3 molecules. *J. Chern. Phys.* 3:136, 1935.

[4] R.P. Feynman, R.B. Leighton, M. Sands. *The Feynman lectures on physics* Vol 3, Reading, MA, Addison-Wesley, 1965.

[5] S. Frauendorf, J. Meng. Tilted rotation of triaxial nuclei. *Nucl. Phys. A* 617:131, 1997.

[6] Q.B. Chen, S.Q. Zhang, P.W. Zhao, R.V. Jolos, J. Meng. Two-dimensional collective Hamiltonian for chiral and wobbling modes. *Phys. Rev. C* 94:044301, 2016.

[7] R. Budaca. Tilted-axis wobbling in odd-mass nuclei. *Phys. Rev. C* 97:024302, 2018.

[8] R. Budaca. Semiclassical description of chiral geometry in triaxial nuclei. *Phys. Rev. C* 98:014303, 2018.

[9] A. Leviatan, D. Shapira. Algebraic benchmark for prolate-oblate coexistence in nuclei. *Phys. Rev. C* 93: 051302(R), 2016.

[10] A.A. Raduta, R. Budaca, C.M. Raduta. Semiclassical description of a triaxial rigid rotor. *Phys. Rev. C* 76:064309, 2007.

[11] A.A. Raduta, R. Poenaru, L.Gr. Ixaru. Semiclassical unified description of wobbling motion in even-even and even-odd nuclei. *Phys. Rev. C* 96:054320, 2017.

[12] S. Bjørnholm, J.E. Lynn, The double-humped fission barrier. *Rev. Mod. Phys.* 52:725, 1980.

[13] T. Nikšić, Z.P. Li, D. Vretenar, L. Próchniak, J. Meng, P. Ring. Beyond the relativistic mean-field approximation. III. Collective Hamiltonian in five dimensions. *Phys. Rev. C* 79:034303, 2009.

[14] R. Budaca, P. Buganu, A.I. Budaca. Bohr model description of the critical point for the first order shape phase transition. *Phys. Lett. B* 776:26-31, 2018.

[15] R. Budaca, P. Buganu, A.I. Budaca. Bohr Model Solution for a Shape Coexisting Potential. *Bulg. J. Phys.* 44:319-325, 2017.

[16] R. Budaca, A.I. Budaca. Coexistence, mixing and fluctuation of nuclear shapes. *EPL* 123:42001, 2018.

[17] S. Frauendorf, J. Meng. Tilted rotation of triaxial nuclei. *Nucl. Phys. A* 617:131, 1997.

[18] H. Taşeli. Accurate computation of the energy spectrum for potentials with multiminima. *Int. J. Quant. Chem.* 46:319 1993.

[19] A. Chandra, K. Bhattacharyya. Stationary anharmonic oscillators in the particle-in-a-box basis: Near-exact results. *Pramana J. Phys.* 43:117 1994.

[20] A. Bohr, B.R. Mottelson. *Nuclear Structure* Vol. 2, Benjamin, Reading, Massachusetts, 1975.

[21] F. Iachello. Analytic description of critical point nuclei in a spherical-axially deformed shape phase transition. *Phys. Rev. Lett.* 87:052502, 2001.

[22] P. Buganu, R. Budaca. Analytical solution for the Davydov-Chaban Hamiltonian with a sextic potential for $\gamma = 30^\circ$. *Phys. Rev. C* 91:014306, 2015.

[23] P. Buganu, R. Budaca. Sextic potential for γ-rigid prolate nuclei. *J. Phys. G: Nucl. Part. Phys.* 42:105106, 2015.

[24] R. Budaca, P. Buganu, M. Chabab, A. Lahbas, M. Oulne. Extended study on a quasi-exact solution of the Bohr Hamiltonian. *Ann. Phys. (NY)* 375:65-90, 2016.

[25] H. Taşeli, A. Zafer. A FourierBessel expansion for solving radial Schrödinger equation in two dimensions. *Int. J. Quant. Chem.* 61:759-768, 1997.

[26] H. Taşeli, A. Zafer. Bessel basis with applications: N-dimensional isotropic polynomial oscillators. *Int. J. Quant. Chem.* 63:935-947, 1997.

[27] H. Taşeli, A. Zafer. Two-sided eigenvalue bounds for the spherically symmetric states of the Schrödinger equation. *J. Comput. Appl. Math.* 95:83-100, 1998.

[28] K.S. Pitzer. The symmetry number and thermodynamic functions for molecules having double minimum vibrations. *J. Chem. Phys.* 7:251-255, 1939.

[29] M.D. Harmony. Tunneling in double-minimum potentials. *Chem. Phys. Lett.* 10:337-340, 1971.