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Towards Nonlinear QRPA Description of States of Multiphonon Origin

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Abstract. We develop a new approach to describe nuclear states of multiphonon origin, motivated by the necessity to describe better nuclear transition of neutrinoless double beta decay. This approach is based on extension of QRPA using the nonlinear phonon operator. Our ultimate goal is to describe all the mother (A, Z), intermediate $(A, Z + 1)$ and daughter nuclear $(A, Z + 2)$ excited states by a single QRPA system. Before that, we develop a nonlinear QRPA within a simplistic model in order to gain better insight. The model is equivalent to the harmonic oscillator, thus exactly solvable. We shall present a novel method to obtain the exact solution by means of a QRPA equation with nonlinear phonon operator formulated separately for every individual excited state.

1 Introduction

For understanding nuclear transition phenomena like, e.g., single or double beta decays, it is crucial to be equipped by a firm description of nuclear structure. As the nuclei are in general systems of tens of nucleons any calculation from first principles is hopeless, and therefore it is necessary to adopt various (often rough) approximations. The Quasiparticle Random Phase Approximation (QRPA) is one of those suitable methods [1–3].

The standard QRPA provides a description of highly correlated ground state and its first excited state. Introducing phonon operator $Q^\dagger = XA^\dagger - YA$ the nucleon-nucleon correlations are taken into account by means of bi-fermion operator A. The phonon operator $Q^\dagger$ creates the first excited state $|1\rangle$ from the ground state $|0\rangle$, which in turn is annihilated by the conjugated phonon operator Q. In order to describe higher excited states usually the multiphonon approach is used. Here the n-th excited state is created by act of $Q^{\dagger n}$ onto $|0\rangle$. In practice it turns out that the multiphonon approach is too naive to get realistic results.

Our work is motivated by the ambition to improve the description of states of multiphonon origin. We present here our achievements in developing a nonlinear extension of QRPA method. The extension is defined by a nonlinear phonon operator $Q_n^\dagger$ which consists of terms of higher powers of $A^\dagger$ and A and thus it is directly able to describe higher excited states. We will refer to the new method as Q_nRPA .

It is useful to test the new ideas within some exactly solvable model. For this purpose the pn-Lipkin model [4–7] is often used which well imitates the structure of the realistic nuclear hamiltonian. In order to simplify the calculation the quasi boson approximation is applied, where the bi-fermion operator A is replaced by purely boson operator B. To maximize the simplicity in this work we study the boson hamiltonian H_B with only up to quadratic terms derived from the pn-Lipkin model.

First, we will demonstrate that the model is equivalent to the harmonic oscillator and we will present the exact solution. Second, we will show that within this particular model, actually, the multiphonon QRPA approach provides exact solution, which is not the case within more realistic models. We will demonstrate the equivalence of the harmonic oscillator and multiphonon QRPA approaches. Third, we will define the new method Q_nRPA and exactly solve the H_B model for the third time. The Q_nRPA will offer a nice insight into the realm of nonlinear phonon operators. We will an outlook towards more realistic application of the Q_nRPA .

2 The Model

Throughout this paper we will present our achievements within the simplistic model defined by

$$H_B = (2\varepsilon + \lambda_1) B^\dagger B + \lambda_2 (B^\dagger B^\dagger + BB) \,, \tag{1}$$

where the operators $B^\dagger$ and B are creation and annihilation boson operator satisfying the algebra $[B, B^\dagger] = 1$. The coefficient ε is a single quasiparticle energy. The coupling constants λ_1 and λ_2 are related to the coupling constants χ' and κ' of the original pn-Lipkin schematic model, see e.g. [5], via

$$\lambda_1 = 2[\chi'(u_p^2 v_n^2 + v_p^2 u_n^2) - \kappa'(u_p^2 u_n^2 + v_p^2 v_n^2)] \,, \tag{2}$$

$$\lambda_2 = 2(\chi' + \kappa') u_p v_p u_n v_n \,, \tag{3}$$

where $u_{p,n} = \sqrt{N_{p,n}/2\Omega}$ and $v_{p,n} = \sqrt{1 - N_{p,n}/2\Omega}$ ($N_{p,n}$ are numbers of protons and neutrons) comes from the Bogoliubov-Valatin transformation of nucleon creation and annihilation operators from the particle into the quasiparticle basis. The schematic model is restricted to the spaces of single-particle states associated with the proton and neutron systems from just a single j-shell with a semidegeneracy $\Omega \equiv j + 1/2$. The simplistic model (1) is derived from the pn-Lipkin model via several approximating steps. After neglecting the scattering terms the hamiltonian acquires the exactly solvable form [5]

$$H_F = \varepsilon C + \lambda_1 A^\dagger A + \lambda_2 (A^\dagger A^\dagger + AA)\,, \tag{4}$$

where the operators C and $A^\dagger$ are the number (proton and neutron) and proton-neutron pair quasiparticle operators, $C \equiv \sum_m (a^\dagger_{pm} a_{pm} + a^\dagger_{nm} a_{nm})$, and $A^\dagger \equiv [a^\dagger_p a^\dagger_n]^{00}$, where a_p and a_n are proton and neutron quasiparticle operators which annihilate the nuclear BCS vacuum $|\rangle$, hence also the operator A annihilates the BCS vacuum, $A\,|\rangle = 0$.

The hamiltonian H_B is obtained from H_F by means of the Marumori boson mapping. In the limit of $\Omega \to \infty$ we get rid of the anharmonic terms, and arrive to the harmonic H_B (1). In this paper we study the model defined by H_B even for finite Ω.

3 The Diagonalization of Hamiltonian

3.1 Fermionic hamiltonain

Thanks to the Pauli exclusion principle the fermion model H_F has a finite number 2Ω of excited states. Exact solution may be found by diagonalization of $(2\Omega+1) \times (2\Omega+1)$ matrix $\langle n'_F|\, H_F\, |n_F\rangle$, whose elements are evaluated in the orthonormal basis of states $|n_F\rangle \propto A^{\dagger n_F}\,|\rangle$, $n_F = 0, \ldots, 2\Omega$. The energies E_n are shown in Figure 1. The eigenstates $|n\rangle$, $n = 0, \ldots, 2\Omega$, are then the linear combinations of basis states $|n_F\rangle$, provided that H_B does not allow to mix even and odd basis states $|n_F\rangle$, thus the even (odd) eigenstates $|n\rangle$ are mixture of the even (odd) basis states only.

3.2 Bosonic hamiltonain

The bosonic model has an infinite number of states as no exclusion principle works for bosons. However, in order to keep the model as an approximation of the fermionic model, one can truncate the tower of states also at the same level of $2\Omega + 1$ states. It is, however, useful to study the behavior of the model in dependence on the number of excited states considered denoted as $n_{\max}$, and also to study the exact solution of the bosonic model with whole infinite tower of states.

The diagonalization of the hamiltonian matrix $\langle n'_B|\, H_B\, |n_B\rangle$ can be performed in the basis of states $|n_B\rangle \propto B^{\dagger n_B}\,|\rangle$, $n_B = 0, \ldots, n_{\max}$. By the symbol $|\rangle$ we denote the bosonic analogue of the BCS vacuum, which is annihilated by the boson operator $B\,|\rangle = 0$.

In Figure 1 we show the comparison of the energy levels of the bosonic and fermionic model. One can appreciate how the energy levels of the bosonic model converge to the exact solution with increasing $n_{\max}$. In the following we will consider only the bosonic model H_B with $n_{\max} = \infty$.

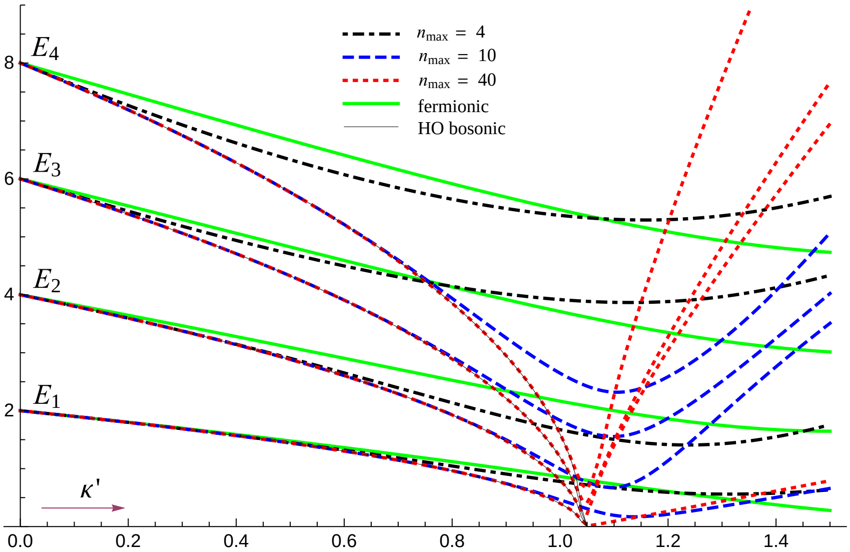

Figure 1. Dependence of energy levels E_n on κ' for $N_p = 4$, $N_n = 6$, $j = 9/2$, $\Omega = 5$, and $\varepsilon = 1$ MeV. The exact solutions for fermionic model H_F and bosonic model H_B (which is equivalent to harmonic oscillator HO) are compared to solutions from diagonalization of H_B with a truncated state basis above $n_{\max}$-th state.

4 Harmonic Oscillator Solution

Contrary to the diagonalization method, in this section we derive an exact solution of the bosonic model H_B, due to considering full tower of boson states, $n_{\max} = \infty$.

We make use of the fact, that H_B describes a harmonic oscillator. Indeed, by transforming the boson creation and annihilation operators into the operators $q = (B^\dagger + B)/\sqrt{2}$, $p = \mathrm{i}(B^\dagger - B)/\sqrt{2}$, we come to the hamiltonian of harmonic oscillator (up to the irrelevant constant term)

$$H_B = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2 - (2\varepsilon + \lambda_1)\,, \tag{5}$$

where $[q, p] = \mathrm{i}$ and

$$\frac{1}{m} = (2\varepsilon + \lambda_1 - 2\lambda_2) \quad \text{and} \quad m\omega^2 = (2\varepsilon + \lambda_1 + 2\lambda_2)\,. \tag{6}$$

The text-book solution of the harmonic oscillator tells us that the frequency ω is the quantum of energy and the energy spectrum is equidistant and given as

$$E_n - E_0 = nE\,, \text{ where } E = \omega = \sqrt{(2\varepsilon + \lambda_1)^2 - 4\lambda_2^2}\,, \tag{7}$$

as it is seen in Figure 1. It is also well know that the hamiltonian of harmonic oscillator can be rewritten as $H_B = (a^\dagger a + \frac{1}{2})\omega$ by means of creation and annihilation operators, which fulfil commutation relation $[a, a^\dagger] = 1$ and $|1\rangle = a^\dagger |0\rangle$, $0 = a|0\rangle$. In terms of the original operators B and $B^\dagger$ we can express

$$a^\dagger = X_{\rm HO} B^\dagger - Y_{\rm HO} B\,, \tag{8}$$

where

$$X_{\rm HO} = \frac{1}{2}\frac{1+m\omega}{\sqrt{m\omega}} = \frac{2\varepsilon + \lambda_1 + E}{\sqrt{2E}\sqrt{2\varepsilon+\lambda_1+E}}\,, \tag{9a}$$

$$Y_{\rm HO} = \frac{1}{2}\frac{1-m\omega}{\sqrt{m\omega}} = \frac{-2\lambda_2}{\sqrt{2E}\sqrt{2\varepsilon+\lambda_1+E}}\,, \tag{9b}$$

and $X_{\rm HO}^2 - Y_{\rm HO}^2 = 1$. This representation of the creation operator $a^\dagger$ is important for comparison of the harmonic oscillator solution with the solution of the standard QRPA, which we are going to discuss in the next section.

5 Standard QRPA and Multiphonon Solution

Within QRPA approach one introduces the phonon operator in the form which is linear in $B^\dagger$ and B

$$Q_1^\dagger = X_1 B^\dagger - Y_1 B\,, \tag{10}$$

where X_1 and Y_1 are called forward- and backward-going free variational amplitudes. The phonon operator creates the first excited state $|1\rangle = Q_1^\dagger |0\rangle$ from the RPA ground state $|0\rangle$, for which one assumes the Ansatz

$$|0\rangle = \mathcal{N} \mathrm{e}^{dB^\dagger B^\dagger} |\rangle\,, \quad \text{where} \quad \mathcal{N}^2 = \sqrt{1-4d^2}\,. \tag{11}$$

The ground state parameter d can be determined from the condition

$$0 \stackrel{!}{=} Q_1 |0\rangle = \mathcal{N}\mathrm{e}^{dB^\dagger B^\dagger}(2dX_1 - Y_1)B^\dagger |\rangle \tag{12}$$

as

$$d = \frac{1}{2}\frac{Y_1}{X_1}\,. \tag{13}$$

The variational amplitudes X_1 and Y_1 satisfy the QRPA equation

$$\begin{pmatrix} \mathcal{A}_1 & \mathcal{B}_1 \\ \mathcal{B}_1 & \mathcal{A}_1 \end{pmatrix} \begin{pmatrix} X_1 \\ Y_1 \end{pmatrix} = E \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X_1 \\ Y_1 \end{pmatrix}, \tag{14}$$

where

$$\mathcal{A}_1 = \langle 0| [B, [H_F, B^\dagger]] |0\rangle = 2\varepsilon + \lambda_1 \tag{15a}$$

$$\mathcal{B}_1 = -\langle 0| [B, [H_F, B]] |0\rangle = 2\lambda_2\,. \tag{15b}$$

The solution (on the right) is obtained by plugging the expressions for $\mathcal{A}_1$ and $\mathcal{B}_1$ (15) into the formal solution (on the left)

$$E = \sqrt{\mathcal{A}_1^2 - \mathcal{B}_1^2} \quad \rightarrow \quad E = \sqrt{(2\varepsilon + \lambda_1)^2 - 4\lambda_2^2}\,, \tag{16a}$$

$$X_1 = \frac{\mathcal{A}_1 + E}{\sqrt{(\mathcal{A}_1 + E)^2 - \mathcal{B}_1^2}} \quad \rightarrow \quad X_1 = \frac{2\varepsilon + \lambda_1 + E}{\sqrt{2E}\sqrt{2\varepsilon + \lambda_1 + E}}\,, \tag{16b}$$

$$Y_1 = \frac{-\mathcal{B}_1}{\sqrt{(\mathcal{A}_1 + E)^2 - \mathcal{B}_1^2}} \quad \rightarrow \quad Y_1 = \frac{-2\lambda_2}{\sqrt{2E}\sqrt{2\varepsilon + \lambda_1 + E}}\,. \tag{16c}$$

which exactly coincides with the harmonic oscillator solution (7) and (9). The RPA amplitudes fulfil completeness and orthogonality relation

$$X_1^2 - Y_1^2 = 1\,, \tag{17}$$

hence $[Q_1, Q_1^\dagger] = 1$. The coefficient of ground state (13) is analytically determined as

$$d \quad = \quad -\frac{(2\varepsilon + \lambda_1) - E}{4\lambda_2}\,. \tag{18}$$

5.1 States of multiphonon origin

The solution of the QRPA equation leads to the phonon operator $Q_1^\dagger$ which coincides with the harmonic oscillator creation operator $a^\dagger$. Then the hamiltonian can be rewritten as $H_B = EQ_1^\dagger Q_1$ up to an irrelevant constant term, which has the standard harmonic oscillator solution

$$E_n - E_0 = nE \quad \text{and} \quad |n\rangle = \frac{1}{\sqrt{n!}} Q_1^{\dagger n} |0\rangle\,. \tag{19}$$

This is nothing but the multiphonon approach within standard QRPA. Within this simplistic model H_B, which is equivalent to the harmonic oscillator, the multiphonon approach gives the exact solution!

For later purpose, let us rewrite the states of multiphonon origin in the form

$$|n\rangle = \frac{1}{\sqrt{n!}} \mathcal{P}_n^\dagger \frac{1}{X_1^n} |0\rangle \quad \text{where} \quad \mathcal{P}_n^\dagger \equiv \sum_{i=0}^{N} c^i f_{n;n-2i} B^{\dagger n-2i}\,, \tag{20}$$

where the upper limit in the sum is $N = \frac{n}{2}$ for even n, and $N = \frac{n-1}{2}$ for odd n. The f-coefficients satisfy the recurrent formula

$$f_{i;j} = f_{i-2;j-2} + (2j+1) f_{i-2;j} + (j+1)(j+2) f_{i-2;j+2}\,, \tag{21}$$

and parameter c is

$$c \equiv -X_1 Y_1\,. \tag{22}$$

For reader's convenience we write explicitly the first several operators $\mathcal{P}_n$:

$$\mathcal{P}_0^\dagger = 1\,, \quad \mathcal{P}_1^\dagger = B^\dagger\,, \quad \mathcal{P}_2^\dagger = (B^{\dagger 2} + c)\,, \quad \mathcal{P}_3^\dagger = (B^{\dagger 3} + 3cB^\dagger)\,,$$
$$\mathcal{P}_4^\dagger = (B^{\dagger 4} + 6cB^{\dagger 2} + 3c^2)\,.$$

6 Q_nRPA with the Nonlinear Phonon Operators for Description of Higher Excited States

Our goal is to define the QRPA procedure providing a QRPA equation of type (14) for every single excited state separately, i.e., to find the form of a phonon operator for which $Q_n^\dagger\,|0\rangle = |n\rangle$ and $Q_n\,|0\rangle = 0$. As the excited states $|n\rangle$ of $n \geq 2$ are of multiphonon origin, the phonon operator $Q_n^\dagger$ should have a nonlinear form

$$Q_n = X_n(B^{\dagger n} + \dots) - Y_n(B^n + \dots)\,. \tag{23}$$

In this section, we present our main achievement of finding the proper phonon operator for all eigenstates of H_B. We are going to show that the nth excited state of the system defined by H_B is excited from the ground state by the phonon operator of the form

$$Q_n^\dagger = X_n\mathcal{P}_n^\dagger - Y_n\mathcal{P}_n\,, \tag{24}$$

where X_n and Y_n are corresponding forward- and backward- going free variational amplitudes. The operator $\mathcal{P}_n$ is defined by (20) as the operator creating the multiphonon states. The important characteristics is that the phonon operator depends just on a single parameter c, which is related to the variational amplitudes of the first excited state according to (22).

For the RPA ground state $|0\rangle$ we try the Ansatz in the same form as for the standard QRPA for the first excited state (11), where we just replace parameter d by d_n, because, at least at first sight, there is no obvious reason that they should coincide. If however by means of QRPA machinery we come to $d = d_n$, then we achieve the common ground state for individual Q_nRPA systems and their mutual consistence.

First of all, we calculate the annihilation condition

$$0 \;\stackrel{!}{=}\; Q_n|0\rangle = X_n\sum_{k=0}^{N}\mathcal{R}_{n;k}B^{\dagger n-2k)}|0\rangle\,, \tag{25}$$

leading to the set of $N+1$ conditions

$$\begin{aligned} 0 \stackrel{!}{=} \mathcal{R}_{n;k} \;\;&\equiv\;\; -c^k f_{n;2(n-k)}(2d_n)^n \\ &\quad + \sum_{i=0}^{k} f_{n;n-2(k-i)}f_{n-2(k-i);n-2k}c^i(2d_n)^{n-k-i}\,. \end{aligned} \tag{26}$$

The solution of the $k=0$ equation provides the expression for the ground state parameter

$$(2d_n)^n = \frac{Y_n}{X_n}\,. \tag{27}$$

This solution can be used in the rest of the equations for $k > 0$ in order to get rid of X_n and Y_n in favor of $(2d)$. The $k = 1$ equation fixes the c parameter

$$c = \frac{(2d_n)}{(2d_n)^2 - 1} \,. \tag{28}$$

and it can be shown that this value satisfies the rest of higher polynomial equations for $k > 1$.

In the nonlinear case the RPA equation (14) has now little bit more complicated form, because the nonzero elements of the norm matrix on the right-hand side are given by $\mathcal{U}_n \equiv \langle 0| [\mathcal{P}_n, \mathcal{P}_n^\dagger] |0\rangle$, which are not equal to one for $n > 1$. However the RPA equation can be easily brought into the standard form by dividing its both sides by $\mathcal{U}_n$. Then the elements of the matrix on the left-hand side are

$$\mathcal{A}_n = \frac{\langle 0| [\mathcal{P}_n, H_B, \mathcal{P}_n^\dagger] |0\rangle}{\langle 0| [\mathcal{P}_n, \mathcal{P}_n^\dagger] |0\rangle} = n\left[(2\varepsilon + \lambda_1) + 2\lambda_2 \frac{(2d_n) - (2d_n)^{2n-1}}{1 - (2d_n)^{2n}}\right], \tag{29}$$

$$\mathcal{B}_n = -\frac{\langle 0| [\mathcal{P}_n, H_B, \mathcal{P}_n] |0\rangle}{\langle 0| [\mathcal{P}_n, \mathcal{P}_n^\dagger] |0\rangle} = 2\lambda_2 n \frac{(2d_n)^{n-1} - (2d_n)^{n+1}}{1 - (2d_n)^{2n}} \,. \tag{30}$$

The standard form of the RPA equation assures that the completeness and orthogonality relation holds in the form

$$X_n^2 - Y_n^2 = 1 \,. \tag{31}$$

The solution of the RPA equation in the standard form is given by (16).

So far, we have expressed everything in terms of the ground-state parameter d_n, which is however still unknown because its expression (27) itself depends on d_n via X_n and Y_n amplitudes. Notice that the expression is different for each n. We can however use (27) as an equation to determine d_n as its root. Hence we would like to solve the equation for d_n

$$(2d_n)^n = \frac{Y_n}{X_n} = \frac{-\mathcal{B}_n}{\mathcal{A}_n + \sqrt{\mathcal{A}_n^2 - \mathcal{B}_n^2}} \,. \tag{32}$$

After plugging (29) and (30) we come to the equation

$$0 \;=\; 2n(2d_n)^{n-1}\left[\lambda_2 + (2\varepsilon + \lambda_1)(2d_n) + \lambda_2(2d_n)^2\right]. \tag{33}$$

For $n > 1$, this equation has 3 solutions independent of n!

$$d_0 = 0\,, \qquad d_\mp = -\frac{(2\varepsilon + \lambda_1) \mp E}{4\lambda_2} \,. \tag{34}$$

Taking the solution d_- as the one defining the true ground state, i.e., the one coinciding with the solution of the standard QRPA with Q_1, we can evaluate the energy of n-th excited state as the solution of QRPA procedure:

$$E_n \;=\; n\sqrt{(2\varepsilon + \lambda_1)^2 - 4\lambda_2^2} = nE\,, \tag{35}$$

and we can see that we are reproducing the harmonic oscillator exact solution once again. Further, the fact that the Q$_n$RPA systems for all n are built above the same ground state, i.e., $d = d_n$ for all n, leads to the relation

$$\frac{Y_n}{X_n} = (2d)^n = \frac{Y_1^n}{X_1^n}\,, \tag{36}$$

which can be used to show that also the parameter c is the same for all n and can be expressed as

$$c = \frac{(2d)}{(2d)^2 - 1} = -X_1 Y_1 \tag{37}$$

in accordance with (22).

We note that using the second nonzero solution of the ground state parameter d_+ leads to exactly the same energies as with the d_- solution. We understand this redundancy of multiple solutions for ground states as an effect of the fact, that by Q$_n$RPA we are solving the solution separately for each excited state. Only if we collect all the Q$_n$RPA solutions together, we come to a single ground state parameter d_- as the Q_1 solution is unique.

7 Simultaneous Q$_n$RPA Description of More Excited States

Very important result of the previous analysis is that the individual Q$_n$RPA systems use a single common ground state $|0\rangle$ given by (11). Therefore it is possible to describe a set of first n excited states simultaneously by a single QRPA system. The nonlinear form of the corresponding phonon operator is

$$Q^\dagger_{\leqslant n} = \sum_{i=1}^{n} Q_i^\dagger = \sum_{i=1}^{n} \left[X_i \mathcal{P}_i^\dagger - Y_i \mathcal{P}_i \right] \,. \tag{38}$$

In fact, it can be shown that one has a great freedom in choosing the form of the $Q^\dagger_{\leqslant n}$ phonon operator. Instead of the operators $\mathcal{P}_i$ one can use other polynomials of B. The RPA equation is in general case rather complicated given in terms of $2n \times 2n$ matrices. However after transforming the phonon operator into the form of (38) it can be shown that the RPA equation breaks to a decoupled equations for individual excited states, i.e., the RPA matrices get a (2×2)-block-diagonal form.

8 Conclusions

Our main goal is to describe better the nuclear structure related to double beta decay. The QRPA method is one of the commonly used.

In our work we are trying to explore the realm of the QRPA extension with nonlinear phonon operator in order to describe better the states of multiphonon origin. For the first stage we have chosen the simple model derived from the pn-Lipkin model after the quasi-boson approximation, which we show to be equivalent to the harmonic oscillator. The simplicity of the model enables us to reach its exact solution. We demonstrate that the exact solution can be fully reproduced by means of nonlinear QRPA method. Actually, one can say that we present a novel way to solve the harmonic oscillator, which might be interesting result per se. We formulate a QRPA system for each excited state individually. While the first excited state is reproduced exactly by standard QRPA with linear phonon operator, the higher excited states requires nonlinear phonon operators. That qualifies the nonlinear phonon operator approach to be relevant and seminal. At the end we shortly discuss the availability of the QRPA systems for simultaneous description of more excited states by a single common phonon operator.

Of course, our ultimate goal is to formulate the extension of the QRPA method for the realistic model and update the database of theoretical predictions for double beta decay nuclear matrix elements. Before that we plan to apply the nonlinear phonon definitions onto more complicated but still exactly solvable models, like pn-Lipkin model given by H_F (4), or like-particle Lipkin model [4, 8].

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