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A new renormalization procedure of the quasiparticle random phase approximation

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The ground state of a many body Hamiltonian considered in the quasiparticle representation is redefined by accounting for the quasiparticle quadrupole pairing interaction. The residual interaction of the newly defined quasiparticles is treated by the quasiparticle random phase approximation (QRPA). Solutions of the resulting equations exhibit specific features. In particular, there is no interaction strength where the first root is vanishing. A comparison with other renormalization methods is presented. Application to a single j-shell allows for the results interpretation by comparing them with those obtained by exact calculations.

Keywords: Deformation; quasiparticles; random phase approximation; renormalization.

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1. Introduction

The big merit of the liquid drop model (LDM) proposed by Bohr and Mottelson[1] is that one defined the concept of rotational bands. Also, some collective properties of spherical nuclei have been nicely described. The main drawback of LDM consists of the fact that it accounts only for the spherical and harmonic motion of the drop, while many experimental data reclaim a nonharmonic picture and, moreover, many nuclei exhibit static deformed shapes. Many phenomenological improvements have been proposed along the time, among which few are to be mentioned: (a) rotation-vibration model;[2] (b) Gneus–Greiner model;[3] (c) generalized collective formalism;[4] (d) coherent state model;[5,6] (e) interacting boson approximation.[7] In parallel, microscopic theories have been formulated, trying to get counterparts of the phenomenological methods and interpret the nuclear collective motion in terms of the single particle motion. Thus, the random phase approximation (RPA) built on the top of either the Hartree–Fock or the BCS ground state (QRPA)[8] provides a collective state which corresponds actually to the one phonon state predicted by the harmonic LDM.[9] Another important result is that of Kumar and Baranger, who calculated the inertial and stiffness parameter microscopically,[10] the potential energy surface leading to some sound nuclear structure interpretation. Based on the RPA ground state, several procedures of accounting for some new correlations, i.e., of going beyond RPA, have been proposed. Such procedures are related with the equations of motion method[11–14] or boson expansion technique.[15,16,18,19]

The RPA method has also been extended to deformed nuclei by using a deformed mean field[20,21] and various two body interactions with the channels of particle-hole (ph), particle-particle (pp) and hole-hole considered on equal footing.[22] To give an example, a fully consistent axially-symmetric deformed Hartree–Fock–Bogoliubov (HFB) + Quasiparticle (QRPA) approach with the D1S Gogny interaction was used in Ref. 24 to study giant resonances in Mg and Si even isotopes. A new method for solving the Skyrme-HFB-QRPA problem in deformed nuclei was reported in Ref. 25. Therein, the Skyrme-HFB-QRPA mean field was calculated in the coordinate-space representation. The formalism was applied for isovector and isoscalar quadrupole modes in spherical ^{20}O and deformed ^{26}Ne nuclei. The effect of deformation on the double beta decay rate[22] has been studied within a deformed pnQRPA.

A common features of all procedures involving QRPA for deformed nuclei is the use of a deformed single particle basis like Nilsson, deformed Woods–Saxon or projected spherical single particle basis,[23] and the quasiparticle-quasiboson approximation is built on the top a static deformed ground state.

A procedure which keeps the appealing harmonic picture of RPA but includes in the definition of the phonon operator new correlations, is obtained by renormalizing the specific equations of motion.[26] This is achieved by considering in the commutation relations of the two quasiparticle operators not only the C-number term, which actually defines the quasi-boson approximation, but also a scalar term which is replaced by its average on the correlated ground state. The average value depends on the RQRPA amplitudes and consequently is to be determined self-consistently together with the RQRPA equations. Thus, the drawback of the standard RPA formalism of collapsing for a critical value of the attractive long range interaction strength, is removed. Indeed, the collective root of the RPA equations goes to zero not for a finite value of the mentioned interaction strength, but only asymptotically. This approach was extended to the proton–neutron Gamow–Teller dipole interaction in Ref. 27. We note that going beyond the quasiboson approximation by considering additional terms in the mutual commutation relations of the quadrupole (or dipole) two quasiparticle operators the Pauli principle, violated by the standard QRPA formalism, is to some extent restored. A more complex procedure was proposed in Ref. 28, where the RPA and BCS equations are simultaneously renormalized. As a consequence the BCS and RPA equations are coupled together and therefore, are to be self-consistently solved.

Vanishing the excitation energy of the collective RPA state corresponds to a phase transition, where the ground state is unstable to adding small contribution. Around this critical interaction, the RPA method is no longer valid. In order to stabilize the ground state it is necessary either to change the mean field for the single particle motion, which results in having deformed single particle orbits, or to renormalize the basic equations.

A distinct renormalization procedure was proposed by Takada in Ref. 29. The author defines two consecutive spherical Bogoliubov–Valatin (BV) transformation for treating the pairing interaction. In the second-order quasiparticle representation, one builds a phonon operator including a scattering term, conventionally called as *attached* field, which allows accounting for nonlinear effects ignored in the standard QRPA. The model was tested, with positive results, for a single j-shell. Note that the second BV transformation is also spherical, i.e., the new quasiparticle operators are tensors of definite rank. Therefore, the new ground state takes account of the paring correlations but not of the quadrupole–quadrupole interaction. The nonlinear effects which renormalize the QRPA are due to the *attached* term and not by deforming the single quasiparticle mean-field.

In the present paper, we propose a new method of renormalizing the QRPA equations. As we shall see, the result for the collective root is that it does not vanish in a critical interaction strength, where the standard QRPA collapses, but reaches a minimum value and moreover the energy increases when a subsequent increase of the strength is performed. The new point of this work is that the mean field is redefined in the quasiparticle picture by including in the ground state the quasiparticle quadrupole pairing correlations. Hence the ground state is redefined by terms of the QQ interaction and not exclusively by pairing correlations, as in Ref. 29. As a result, both the new quasiparticles and the new QRPA solutions are deformed.

The project sketched above will be described according to the following plan. In Sec. 2 the model Hamiltonian is presented. For the sake of completeness, the results for the standard BCS and QRPA equations are briefly described. Section 3 is devoted to the deformed quasiparticles or, in other words, to the second-order BCS approach. The new BCS and QRPA equations are analytically derived. In Sec. 4, the formalism is numerically applied to a single j-shell. The new method is compared with the HFB formalism in Sec. 5. The final conclusions are drawn in Sec. 6.

2. The Model Hamiltonian

We consider a system of nucleons described by a many body Hamiltonian consisting of the spherical mean field term, the pairing and the quadrupole–quadrupole two body interactions. Written in second quantization, this has the form:

$$H = \sum_{\alpha}(\epsilon_a - \lambda)c^{\dagger}_{\alpha}c_{\alpha} - \frac{G}{4}P^{\dagger}P - \frac{X}{4}\sum_{\mu}Q_{2\mu}Q_{2-\mu}(-)^{\mu}, \tag{2.1}$$

where $P^\dagger$ and Q denote the pairing and quadrupole operator, respectively

$$P^\dagger = \sum_\alpha c^\dagger_\alpha c^\dagger_{-\alpha}(-)^{j_\alpha - m_\alpha},$$
$$Q_{2\mu} = \sum_{\alpha,\beta}\langle\alpha|r^2Y_2|\beta\rangle c^\dagger_\alpha c_\beta \equiv \sum_{a,b,\mu} q_{ab}(c^\dagger_a c_b)_{2\mu}, \tag{2.2}$$
$$q_{ab} = \frac{\hat{j}_a}{\hat{2}}\langle a\|r^2Y_2\|b\rangle, \quad \text{with } \hat{j}_a = \sqrt{2j_a+1}.$$

The ph quadrupole operator is defined as

$$(c^\dagger_a c_b)_{2\mu} = \sum_{m_\alpha,m_\beta} C^{j_a j_b 2}_{m_\alpha -m_\beta \mu} c^\dagger_\alpha c_\beta (-)^{j_b - m_\beta}. \tag{2.3}$$

The second quantization is used within the spherical shell model basis $|\alpha\rangle = |a, m_\alpha\rangle = |n_a l_a j_a m_\alpha\rangle$. Thus, the creation (annihilation) operator of one particle in the state $|\alpha\rangle$ is denoted by $c^\dagger_\alpha(c_\alpha)$. We also used the notation $|-\alpha\rangle = |a, -m_\alpha\rangle$.

The sum of the first two terms in Eq. (2.1) is quasidiagonalized by passing to the quasiparticle representation defined by the BV transformation

$$\begin{aligned} a^\dagger_\alpha &= U_\alpha c^\dagger_\alpha - V_a s_\alpha c_\alpha, \\ a_\alpha &= U_a c_\alpha - V_a s_\alpha c^\dagger_{-\alpha}, \quad \text{with } s_\alpha = (-)^{j_a - m_\alpha}. \end{aligned} \tag{2.4}$$

The quasiparticle vacuum state will be hereafter denoted by $|\mathrm{BCS}\rangle$. In the new representation up to an additive constant, the Hamiltonian is

$$H = \sum_\alpha E_a a^\dagger_\alpha a_\alpha - \frac{X}{4}\sum_\mu Q_{2\mu}Q_{2,-\mu}(-)^\mu, \tag{2.5}$$

where E_a denotes the quasiparticle energy for the state characterized by the set of quantum numbers "α", while the quadrupole operators can be expressed in terms of two quasiparticle and quasiparticle quadrupole density operators

$$\begin{aligned} Q_{2\mu} &= \sum_{a\le b} q_{ab}[\xi_{ab}(A^\dagger_{2\mu}(ab) + A_{2-\mu}(ab)(-)^\mu) \\ &\quad + \eta_{ab}(B^\dagger_{2\mu}(ab) + B_{2-\mu}(ab)(-)^\mu)], \\ A^\dagger_{2\mu}(ab) &= \frac{1}{\sqrt{1+\delta_{ab}}}\sum_{m_\alpha,m_\beta} C^{j_a\ j_b\ 2}_{m_\alpha m_\beta \mu} a^\dagger_\alpha a^\dagger_\beta, \\ B^\dagger_{2\mu}(ab) &= \sum_{m_\alpha,m_\beta} C^{j_a\ j_b\ 2}_{m_\alpha -m_\beta \mu} a^\dagger_\alpha a_\beta s_\beta, \\ A_{2\mu}(ab) &= (A^\dagger_{2\mu}(ab))^\dagger; \quad B_{2\mu}(ab) = (B^\dagger_{2\mu}(ab))^\dagger, \\ \xi_{ab} &= \frac{1}{\sqrt{1+\delta_{ab}}}(U_aV_b + U_bV_a), \quad \eta_{ab} = \frac{1}{1+\delta_{ab}}(U_aU_b - V_aV_b). \end{aligned} \tag{2.6}$$

In deriving the expression of the quadrupole operator in the quasiparticle representation, some symmetry properties were used

$$\begin{aligned} A^{\dagger}_{2\mu}(ba) &= (-)^{j_a-j_b}A^{\dagger}_{2\mu}(ab); \quad A_{2\mu}(ba) = (-)^{j_a-j_b}A_{2\mu}(ab), \\ B^{\dagger}_{2\mu}(ba) &= (-)^{j_a-j_b}B_{2-\mu}(ab)(-)^{\mu}; \quad B_{2\mu}(ba) = (-)^{j_a-j_b}B^{\dagger}_{2-\mu}(ab)(-)^{\mu}, \\ q_{ba} &= (-)^{j_a-j_b}q_{ab}. \end{aligned} \tag{2.7}$$

The quasiparticle many body Hamiltonian is treated within the Random Phase Approximation (QRPA) formalism. Thus, one defines a phonon operator

$$C^{\dagger}_{2\mu} = \sum [X(ab)A^{\dagger}_{2\mu}(ab) - Y(ab)A_{2-\mu}(ab)(-)^{\mu}] \tag{2.8}$$

with the amplitudes $X(ab)$ and $Y(ab)$ determined such that the following equations are fulfilled:

$$[H, C^{\dagger}_{2\mu}] = \omega C^{\dagger}_{2\mu}, \quad [C_{2\mu}, C^{\dagger}_{2\mu'}] = \delta_{\mu,\mu'}. \tag{2.9}$$

The first equation yields for the phonon amplitudes the so-called QRPA equations

$$\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ -\mathcal{B}^* & -\mathcal{A}^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \omega \begin{pmatrix} X \\ Y \end{pmatrix}. \tag{2.10}$$

This is a homogeneous system of linear equations determining the phonon amplitudes up to a multiplicative factor, fixed by the second equation (2.9) which gives:

$$\sum_{ab} [|X(ab)|^2 - |Y(ab)|^2] = 1. \tag{2.11}$$

The matrices involved in Eq. (2.9) have the expressions

$$\begin{aligned} \mathcal{A}_{ab,a'b'} &= (E_a + E_b)\delta_{a,a'}\delta_{b,b'} - \frac{X}{2} r_{ab} r_{a'b'}, \\ \mathcal{B}_{ab,a'b'} &= -\frac{X}{2} r_{ab} r_{a'b'}, \quad \text{with } r_{ab} = q_{ab}\xi_{ab}. \end{aligned} \tag{2.12}$$

Once the QRPA equations are solved, the phonon space is defined. Thus, the vacuum state denoted by $|\mathrm{RPA}\rangle$ is the ground state, while the excited states are multi-phonon excitations of $|\mathrm{RPA}\rangle$. Since the two body interaction is of a separable form, the QRPA equations provide a dispersion equation for the excitation energies and analytical expressions for the phonon amplitudes. By inspecting of these expressions, one finds that the first excited state corresponds to an energy smaller than the minimal two quasiparticle energy and has a collective character. Due to the attractive nature of the two body interaction, the collective state energy is decreasing when the interaction strength X is increased. Consequently, for a critical value of X the phonon energy is vanishing and the phonon operator cannot be determined. This situation defines the breaking down point of the QRPA approach. To avoid this regime, the mean field for the single particle motion should be re-defined, which results in renormalizing the ground state energy such that the collective state has a positive energy. Concretely, the spherical shell model single particle basis is to be replaced with the Nilsson single particle basis. Another way to remove the QRPA breaking down is to define a new phonon operator by going beyond the QRPA approach, which is actually based on the quasiboson approximation of the two quasiparticle quadrupole operators $A^{\dagger}_{2\mu}$ and $A_{2\mu}$. The quasiboson commutation equations have been corrected by retaining from the exact expression not only the constant term but also the scalar one, which is considered in the average. This average is determined self-consistently together with the QRPA solution and, consequently, the collective root energy goes to zero only asymptotically. In the next section, we formulate a new method to renormalize the ground state energy.

3. Deformed Quasiparticles

Here, we study the BCS ground state excitation

$$\begin{aligned} |\widetilde{\mathrm{BCS}}\rangle &= e^{T}|\mathrm{BCS}\rangle, \text{with} \\ T &= z_{\alpha}a^{\dagger}_{\alpha}a^{\dagger}_{-\alpha} - z^{*}_{\alpha}a_{-\alpha}a_{\alpha}s_{\alpha}. \end{aligned} \tag{3.1}$$

In what follows, it is useful to employ the polar representation of the parameters z_{α}:

$$z_{\alpha} = \rho_{\alpha}e^{i\varphi_{\alpha}}. \tag{3.2}$$

The images of the quasiparticle operators through the afore-defined transformation, are

$$\begin{aligned} d^{\dagger}_{\alpha} &= e^{T}a^{\dagger}_{\alpha}e^{-T} = a^{\dagger}_{\alpha}\cos(2\rho_{\alpha}) - a_{-\alpha}s_{\alpha}\sin(2\rho_{\alpha})e^{-i\varphi_{\alpha}}, \\ d_{\alpha} &= e^{T}a_{\alpha}e^{-T} = a_{\alpha}\cos(2\rho_{\alpha}) - a^{\dagger}_{-\alpha}s_{\alpha}\sin(2\rho_{\alpha})e^{i\varphi_{\alpha}}. \end{aligned} \tag{3.3}$$

With the obvious notations:

$$u_{\alpha} = \cos(2\rho_{\alpha}); \quad v_{\alpha} = \sin(2\rho_{\alpha})e^{-i\varphi_{\alpha}}, \tag{3.4}$$

we recognize the BV transformation for the quasiparticle operators. The transformation parameters u_{α} and v_{α} satisfy the equation:

$$u^{2}_{\alpha} + |v_{\alpha}|^{2} = 1, \tag{3.5}$$

which reflects the fermionic character of the new quasiparticle operators $d^{\dagger}_{\alpha}$ and d_{α}. We note that the transformed state $|\widetilde{\mathrm{BCS}}\rangle$ is vacuum state for the quasiparticle annihilation operators d_{α}. It is worth mentioning that due to the transformation dependence on the magnetic quantum number m_{α}, the new quasiparticle operators are tensors of rank j_{a} with indefinite projection. In this respect, one can assert that the newly defined quasiparticles are deformed operators.

The parameters u_{α} and v_{α} may be viewed as classical coordinates depending on time. Moreover, considering the polar representation, the phase φ_{α}, defining the coefficient v_{α}, has the meaning of a generalized linear momentum. Consequently, since we are concerned with the static properties of the new BV transformation coefficients, it is reasonable to consider vanishing phases φ_{α}.

In what follows, we try to determine the parameters u_α and v_α such that the transformed state $|\widetilde{\mathrm{BCS}}\rangle$ becomes the true ground state of the many body system under consideration, i.e., it corresponds to an energy lower than that associated with $|\mathrm{BCS}\rangle$. The new ground state is a deformed function, which is reflected by the nonvanishing value of the expected quadrupole moment:

$$\langle\widetilde{\mathrm{BCS}}|Q_{20}|\widetilde{\mathrm{BCS}}\rangle = \sqrt{20}\sum_{a,m_\alpha>0}\frac{q_{aa}}{\hat{j}_a}C^{j_a 2 j_a}_{m_\alpha 0 m_\alpha}(\xi_{aa}(u_{-\alpha}v_\alpha + u_\alpha v_{-\alpha}) + \eta_{aa}(v_\alpha^2 + v_{-\alpha}^2)) \equiv q_0. \tag{3.6}$$

The last part of the above relation expresses the fact that the state $|\widetilde{\mathrm{BCS}}\rangle$ has a definite quadrupole deformation q_0. The average value of H with the deformed state $|\widetilde{\mathrm{BCS}}\rangle$ is

$$\begin{aligned}\mathcal{E}' &= \langle\widetilde{\mathrm{BCS}}|H|\widetilde{\mathrm{BCS}}\rangle \\ &= \sum_\alpha E_a v_\alpha^2 - \frac{\Delta_{20}^2}{X} - \frac{X}{2}\sum_{a,b,m_\alpha}[q_{ab}C^{j_a j_b 2}_{m_\alpha -m_\alpha 0} \\ &\quad\times(\xi_{ab}(u_{-\alpha}u_{b,m_\alpha} - v_\alpha v_{b,-m_\alpha}) + \eta_{ab}(u_{b,m_\alpha}v_\alpha + u_{-\alpha}v_{b,-m_\alpha}))]^2,\end{aligned} \tag{3.7}$$

where we denoted:

$$\Delta_{20} = \frac{X}{2}\langle\widetilde{\mathrm{BCS}}|Q_{20}|\widetilde{\mathrm{BCS}}\rangle. \tag{3.8}$$

Note that, the last term of Eq. (3.7) is provided by the average of the quasiparticle terms of the type $d_\alpha d_{b,m_\alpha} d^\dagger_{b',m_{\alpha'}} d^\dagger_{-\alpha'}$. However, such terms will be treated at the QRPA level, i.e., at a later stage. Due to this reason, hereafter, the mentioned term from Eq. (3.7) will be neglected.

In what follows, we shall look for the stationary points of the function:

$$\mathcal{E} = \sum_\alpha E_a v_\alpha^2 - \frac{\Delta_{20}^2}{X} - \sum_\alpha \mu_\alpha(u_\alpha^2 + v_\alpha^2 - 1) \tag{3.9}$$

with μ_α denoting the Lagrange multiplier corresponding to the restriction (3.5). These are solutions of the equations obtained by vanishing the first derivatives of $\mathcal{E}$ with respect to the parameters u_α and v_α, defining the BV quasiparticle transformation. Eliminating the Lagrange multipliers, one arrives at:

$$\Delta_{20}\xi_{aa}\bar{Q}_{\alpha\alpha}(u_\alpha u_{-\alpha} - v_\alpha v_{-\alpha}) - (E_a - 2\Delta_{20}\eta_{aa}\bar{Q}_{\alpha\alpha})u_\alpha v_\alpha = 0, \tag{3.10}$$

where the following notation has been used:

$$\bar{Q}_{\alpha\alpha} = \frac{\hat{2}}{\hat{j}_a}C^{j_a 2 j_a}_{m_\alpha 0 m_\alpha}q_{aa}. \tag{3.11}$$

We remark that the above equation is invariant to the change $\alpha \to -\alpha$. This suggests that the solutions of the above equation satisfy:

$$u_\alpha = u_{-\alpha}, \quad v_\alpha = v_{-\alpha}. \tag{3.12}$$

Thus, the occupation probabilities acquire the expressions:

$$\begin{pmatrix} v_\alpha^2 \\ u_\alpha^2 \end{pmatrix} = \frac{1}{2}\left(1 \mp \frac{E_a - 2\Delta_{20}\eta_{aa}\bar{Q}_{\alpha\alpha}}{\sqrt{(E_a - 2\Delta_{20}\eta_{aa}\bar{Q}_{\alpha\alpha})^2 + (2\Delta_{20}\xi_{aa}\bar{Q}_{\alpha\alpha})^2}}\right). \tag{3.13}$$

It is interesting to note that by the quadrupole moment restriction and

$$\Delta_{20} = \frac{X}{2} q_0, \tag{3.14}$$

Eq. (3.13) fully determines the parameters v_α and u_α. With the notations:

$$\begin{aligned} \bar{E}_\alpha &= E_a - 2\Delta_{20}\eta_{aa}\bar{Q}_{\alpha\alpha}, \quad \delta_\alpha = 2\Delta_{20}\xi_{aa}\bar{Q}_{\alpha\alpha}, \\ e_\alpha &= \sqrt{\bar{E}_\alpha^2 + \delta_\alpha^2}, \end{aligned} \tag{3.15}$$

one obtains a more transparent expression for the BV transformation coefficients

$$\begin{pmatrix} v_\alpha^2 \\ u_\alpha^2 \end{pmatrix} = \frac{1}{2}\left(1 \mp \frac{\bar{E}_\alpha}{e_\alpha}\right). \tag{3.16}$$

The quantity e_α has the significance of the second-order quasiparticle energy, i.e., the energy corresponding to the deformed quasiparticle state $|\alpha\rangle = d_\alpha^\dagger|\widetilde{\mathrm{BCS}}\rangle$. Further, we shall define a phonon operator

$$\Gamma^\dagger = \sum_{ab,m_\alpha} (X_{m_\alpha}^{ab} d_\alpha^\dagger d_{b,-m_\alpha}^\dagger - Y_{m_\alpha}^{ab} d_{b,-m_\alpha} d_\alpha), \tag{3.17}$$

such that it obeys the equations

$$[H, \Gamma^\dagger] = \omega\Gamma^\dagger, \quad [\Gamma, \Gamma^\dagger] = 1. \tag{3.18}$$

In terms of the new quasiparticles, the model Hamiltonian is

$$\begin{aligned} H = \sum_\alpha e_\alpha d_\alpha^\dagger d_\alpha - \frac{X}{4} \sum_{a,b,m_\alpha} Q_{m_\alpha}^{ab} (d_\alpha^\dagger d_{b,-m_\alpha}^\dagger + d_{b,-m_\alpha} d_\alpha) \\ \times \sum_{a',b',m_{\alpha'}} Q_{m'_\alpha}^{a'b'} (d_{\alpha'}^\dagger d_{b',-m_{\alpha'}}^\dagger + d_{b',-m_{\alpha'}} d_{\alpha'}) \end{aligned} \tag{3.19}$$

with the notation

$$\begin{aligned} Q_{m_\alpha}^{ab} &= C_{m_\alpha\, -m_\alpha\, 0}^{j_a\ j_b\ 2} q_{ab}[\xi_{ab}(u_\alpha u_{b,-m_\alpha} - (-1)^{j_a - j_b} v_{-\alpha} v_{b,m_\alpha}) \\ &\quad + \eta_{ab}(u_{-\alpha} v_{b,-m_\alpha} + v_\alpha u_{b,m_\alpha})]. \end{aligned} \tag{3.20}$$

The amplitudes $X_{m_\alpha}^{ab}$ and $Y_{m_\alpha}^{ab}$ are determined by the QRPA equations, which are of a similar form as those given by Eq. (2.10), and the normalization condition:

$$2 \sum_{a,b,m_\alpha} [(X_{m_\alpha}^{ab})^2 - (Y_{m_\alpha}^{ab})^2] = 1. \tag{3.21}$$

The matrices involved in the QRPA equations have the expressions

$$\begin{aligned} \mathcal{A}_{m_\alpha;m_{\alpha'}}^{ab;a'b'} &= (e_\alpha + e_{b,m_\alpha})\delta aa'\delta_{bb'}\delta_{m_\alpha m_{\alpha'}} - XQ_{m_\alpha}^{ab} Q_{m_{\alpha'}}^{a'b'}, \\ \mathcal{B}_{m_\alpha;m_{\alpha'}}^{ab;a'b'} &= -XQ_{m_\alpha}^{ab} Q_{m_{\alpha'}}^{a'b'}. \end{aligned} \tag{3.22}$$

Since the two body interaction involved in H is separable, the compatibility condition for the QRPA equations may be brought to the form of a dispersion equation, while the phonon amplitudes are analytically expressed. Now, it is worth noting that both the QRPA and the deformed BCS equations involve the factors η_{ab}. This reflects the fact that the terms $B^{\dagger}_{2\mu}$ and $B_{2-\mu}(-)^{\mu}$ of the Hamiltonian expressed in terms of spherical quasiparticles, contribute to the mentioned equations. This feature contrasts the standard QRPA equations, which ignore the scattering terms.

4. The Case of a Single *j*-Shell

The essential features of the QRPA formalism with a multi-shell calculations can be recovered by restricting the single particle space to a single j. Since here we are not interested in quantitative details, but rather in underlying the main virtues of the proposed formalism, we consider the numerical application for the single j case. Thus, one considers a system of $N = 10$ nucleons moving in the spherical shell model state $j = i_{13/2}$ and described by the corresponding many body Hamiltonian (2.1). We present separately the spherical and deformed QRPA results.

4.1. *Results for QRPA built on the top of the first order BCS*

The occupation probabilities are

$$V^2 = \frac{N}{2\Omega}, \quad U^2 = 1 - \frac{N}{2\Omega}. \tag{4.1}$$

For the sake of simplifying the notation, the low indices of U and V, specifying the chosen single j are omitted. The state semi-degeneracy is denoted by Ω. Neglecting the term $G\Omega V^4$ accounting for the renormalization of the single particle energy due to the residual interaction, the BCS ground state energy is

$$E = 2\epsilon\Omega V^2 - \frac{\Delta^2}{G} = 2\epsilon\Omega V^2 - G\Omega^2 V^2(1 - V^2). \tag{4.2}$$

We recall that G is defined by Eq. (2.1) as the strength of the pairing interaction. Here, the Fermi level energy is set equal to zero. The condition of minimum energy leads to:

$$V^2 = \frac{1}{2}\left(1 - \frac{2\epsilon}{G\Omega}\right). \tag{4.3}$$

This expression is consistent with Eq. (4.1) if the single particle energy is

$$\epsilon = \frac{G\Omega}{2}\left(1 - \frac{N}{\Omega}\right). \tag{4.4}$$

Equation (4.3) gives for the quasiparticle energy

$$E_q = \frac{G\Omega}{2}. \tag{4.5}$$

In our application, we took $G = 0.4\,\mathrm{MeV}$, which results of having $E_q = 1.4\,\mathrm{MeV}$. The compatibility condition for the QRPA equations reads

$$\omega^2 = 4E_q^2 - 2Xq_{jj}^2\xi_{jj}^2. \tag{4.6}$$

The positive root of this equation is

$$\omega = \left[G^2\Omega^2 - \frac{8}{5}\Omega X(\langle j||r^2Y_2||j\rangle)^2\frac{N}{2\Omega}\left(1 - \frac{N}{2\Omega}\right)\right]^{1/2}. \tag{4.7}$$

The QRPA energy is plotted in Fig. 1 as function of X. From this figure, we notice that for $X = 0$ the mode energy is equal to twice the quasiparticle energy, while for $X \approx 1.82\ 10^{-3}\,\mathrm{MeV\,fm^{-4}}$ this is vanishing. Within this interval the function is monotonically decreasing. The vanishing mode energy reclaims a breaking down for the QRPA approach. In next section, we describe a method of recovering the validity of the QRPA approach.

4.2. *The study of QRPA for the quadrupole pairing correlated quasiparticles*

Switching on the quadrupole pairing correlations for the spherical quasiparticles, we have

$$\begin{aligned}
\bar{E}_m &= E_q - \frac{X}{2}q_0(U^2 - V^2)\langle j||r^2Y_2||j\rangle C^{j2j}_{m0m},\\
\delta_m &= Xq_0\sqrt{2}UV\langle j||r^2Y_2||j\rangle C^{j2j}_{m0m}, \qquad (4.8)\\
e_m &= \sqrt{\bar{E}_m^2 + \delta_m^2},
\end{aligned}$$

$$v_m^2 = \frac{1}{2}\left(1 - \frac{\bar{E}_m}{e_m}\right), \quad u_m^2 = 1 - v_m^2. \tag{4.9}$$

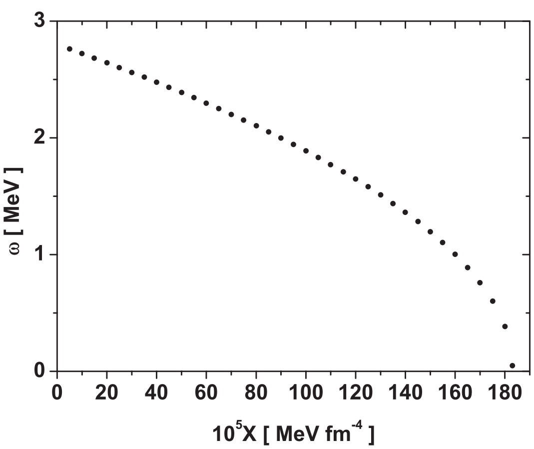

Fig. 1. The spherical QRPA energy as function of the quadrupole–quadrupole interaction strength for the case of a single shell, $j = i_{13/2}$.

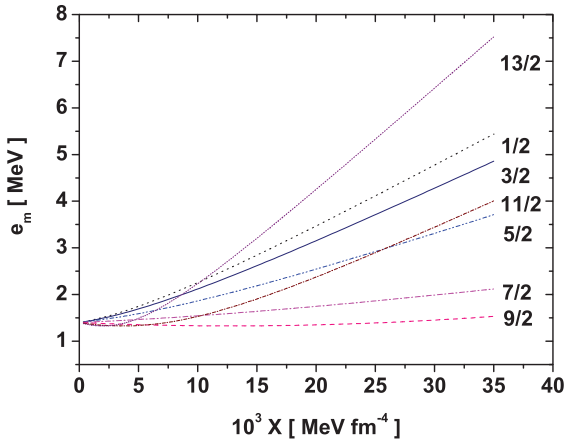

Fig. 2. The deformed quasiparticle energies for the $j = i_{13/2}$ multiplet.

Numerical results correspond to $q_0 = 30\,\text{fm}^2$. One notices that the newly defined quasiparticle energy depends on the magnetic quantum number "m". The split, caused by the quadrupole moment of the single particle state $|jm\rangle$, is shown in Fig. 2 as function of X, the strength of the QQ interaction. Another peculiarity for the second-order BCS ground state is that the average number of quasiparticles is not vanishing.

$$\langle\widetilde{\mathrm{BCS}}|\hat{N}_q|\widetilde{\mathrm{BCS}}\rangle = \sum_m v_m^2, \tag{4.10}$$

where the quasiparticle number operator is denoted by

$$\hat{N}_q = \sum_\alpha a_\alpha^\dagger a_\alpha. \tag{4.11}$$

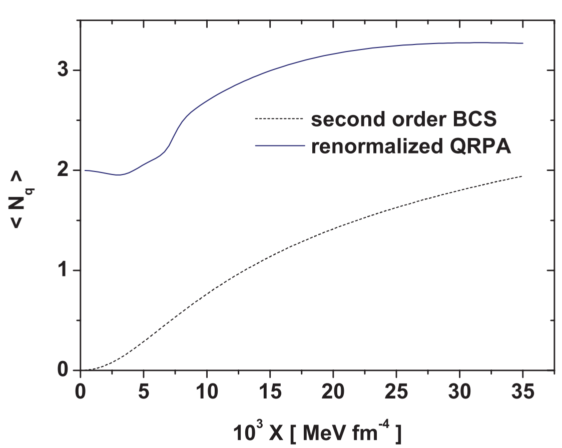

Fig. 3. The average number of quasiparticles in the second-order BCS state, $|\widetilde{\mathrm{BCS}}\rangle$.

The dependence of the quasiparticle average number on the interaction strength is shown in Fig. 3. Note that the larger the strength X, the larger the quasiparticle averaged number. This result also implies the presence of quasiparticles in the QRPA ground state. Indeed, denoting by $|\mathrm{RQRPA}\rangle$ the RQRPA ground state, one can prove that

$$\langle|\hat{N}_q|\rangle = \sum_m v_m^2 + 2\sum_{m,k}(u_m^2 - v_m^2)((X_m(k))^2 + (Y_m(k))^2), \tag{4.12}$$

where the argument k of the amplitudes X and Y labels the roots of the RQRPA equations. In Fig. 3, the average number of quasiparticles is calculated by restricting the second sum of the above equation to $k = 1$. This is consistent with the fact that the other calculations referred to the first excited states. Adding the contributions of the higher roots amplitudes would increase the average quasiparticle number. The nonmonotonic structure in the interval [0,7.5]MeV of $\langle\hat{N}_q\rangle$ corresponds to the first branch of the first excited RQRPA energy shown in Fig. 4.

In order to write the QRPA equation, we need to know the matrix $Q^{ab}_{m_\alpha}$ defined by Eq. (3.20). In the case of a single j-shell one obtains:

$$Q^{jj}_m = (-)^{j-m} C^{j2j}_{m0m} \langle j||r^2Y_2||j\rangle(\sqrt{2}UV(u_m^2 - v_m^2) + (U^2 - V^2)u_m v_m). \tag{4.13}$$

The compatibility condition for the QRPA equations can be written under the form of a dispersion equation:

$$1 = X\sum_{m>0}\frac{(Q^{jj}_m)^2 4e_m}{4e_m^2 - \omega^2}. \tag{4.14}$$

For the chosen value of j, there are seven solutions for ω denoted by $\omega(m)$ and ordered as

$$\omega(1) < \omega(2) < \cdots < \omega(7). \tag{4.15}$$

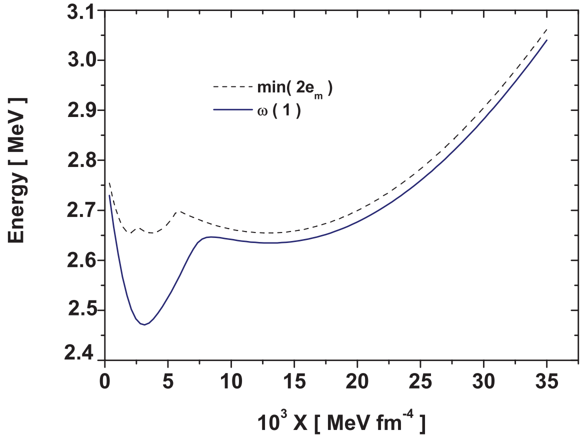

Fig. 4. The first QRPA equation root as a function of the QQ interaction strength. The minimal two quasiparticle energies are also presented as a function of X.

The first root has a collective character since several quasiparticle pairs contribute to the phonon operator. Note that $\omega(1)$ is smaller, in magnitude, than the minimal two quasiparticle energy, $\min(2e_m)$. The two afore-compared quantities are represented as function of the long range interaction strength X, in Fig. 4. We note that $\omega(1)$ is no longer a monotonic function of X. There are, however, two intervals of different monotony. On the first interval $\omega(1)$ is decreasing, reaches a minimum and then it increases in the second interval. The minimum value is reached for X close to the value where the spherical phonon energy is vanishing. Due to this behavior, in the second interval there is no breaking down for the QRPA approach. Due to the specific dependence of the terms $2e_m$ and Q_m^{jj} on the strength X, $\omega(1)$ behaves as if from the minimum point on, the effective two body interaction changes its attractive nature to a repulsive one. Also, it is worth noting that in the region around the minimum X the difference $\min(2e_m) - \omega(1)$ is large comparing it with the values corresponding to the X from the complementary interval. This feature reflects the collective property[30] of the corresponding phonon state. We may say that the maximal collectivity is reached for the critical value of X. Around this point the spherical and deformed systems might be described in a unified fashion by using a spherical single particle basis.

Now, we would like to mention that in Ref. 29 a similar approach was used as to treat the many body Hamiltonian with a spherical shell model mean field, a pairing plus a $Q \cdot Q$ interaction. However, between our approach and that proposed in the quoted reference, there are several essential differences which will be listed below:

(1) The second BV used in Ref. 29 is specific to a spherical BCS formalism, the new quasiparticle operators being tensors of definite rank and definite projection on the axis OZ. Such a transformation preserves the rotational symmetry and consequently the transformed Hamiltonian behaves like a scalar under rotation transformations. The new BCS ground state is a function of vanishing angular momentum and the corrected quasiparticle energy does not depend on the magnetic quantum number. By contrast, in our case the BV transformation characterizes the quasiparticle quadrupole pairing interaction, which results in having a deformed quasiparticle operator with the u and v coefficients baring the indices α and not only a. The vacuum state for the newly defined quasiparticle operators is a deformed wave function. Since the BV transformation breaks the rotation symmetry the Hamiltonian written in terms of the new operators is not a scalar operator.

(2) The quasiparticle states are deformed in our formalism, while in Ref. 29, they have definite angular momentum and angular momentum projection on the axis OZ.

(3) The second BCS equations (3.13) and the consistency condition (3.6) are to be simultaneously considered, which allows us to have the occupation probabilities fully determined before passing to the QRPA treatment. Thus, the phonon amplitudes are involved neither in the BCS equations nor in the consistency

restriction. However, in the case that the strength of the $Q \cdot Q$ interaction, X, is fixed by fitting the lowest QRPA root to the experimental energy for the lowest 2^+ state, then the two sets of equations, BCS and QRPA, are coupled by the interaction strength.

(4) In Ref. 29, the renormalization is caused by the so called "attached field". Indeed, the Hamiltonian terms not included in the standard QRPA but taken into account within the renormalization procedure are involved in the equation relating the amplitudes of the scattering ("attached" term) and the two quasiparticle terms, composing the phonon operator. In our method, the renormalization is produced due the deformation induced by the BV transformation and moreover there is no need of an "attached" field.

(5) The QRPA treatment is defined within a large single-quasiparticle deformed space while in Ref. 29 within a space of spherical single-quasiparticle space, of much lower dimension.

(6) The features mentioned above are reflected in the results for the single j space. Indeed, the energy for the new quasiparticles are split over the quantum number m; see Fig. 2.

(7) The QRPA dispersion equation has Ω solutions and not only one as happens in Ref. 29.

(8) The energy eigenvalue for the case when the full self-consistency problem is solved, is a continuous decreasing function of the interaction strength while in our case the mentioned curve exhibits a minimum.

(9) The QRPA states described in Ref. 29 are eigenstates of $\hat{J}^2$ and J_z, while in our case only "K" is a good quantum number. If an angular momentum projection is subsequently performed, then to each state one associates a finite rotational band. On the other hand, the formalism of Ref. 29 cannot be used for rotational bands which, as a matter of fact, is an attribute of deformed systems. Here, the renormalized QRPA states have $K = 0$. However, Eqs. (3.17)–(3.22) can be easily extended to an arbitrary K.

Concluding, the two renormalization procedures are applicable to different nuclear systems, one with and one without rotational symmetry.

4.3. *Exact results*

The application to a single j case is justified by the fact that the main features of the low lying states provided by a multi-shell calculation are recovered with small computational efforts. As a matter of fact, this is clearly shown by the results described above. On the other hand, the eigenvalues of a PP + QQ Hamiltonian in a single j-shell can be exactly calculated. Therefore, comparing the exact results with those obtained through sophisticated many body approaches one can judge upon the correctness of the employed approximations.[31] Of course, recalling the relation between single and multi-shell reflected in their common features, one hopes that the conclusion regarding the approximation validity drawn for single j-shell may

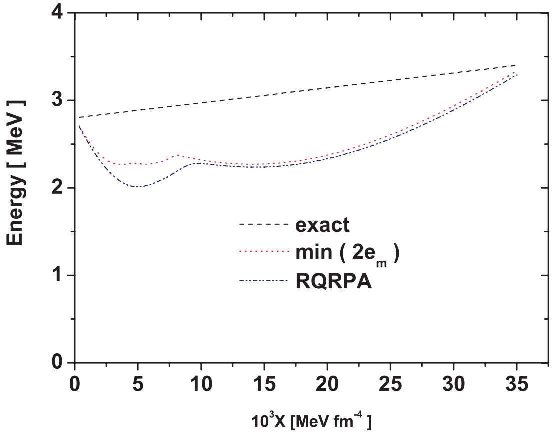

Fig. 5. The first excited state energies predicted by the renormalized QRPA are compared with the energy of the first 2^+ state, given by the exact calculation in the case of two nucleons moving in the single shell $j = 13/2$. The minimal two quasiparticle energies are also presented. The three sets of energies are plotted as function of the QQ interaction strength, X. The RQRPA results correspond to $q_0 = 56\,\text{fm}^2$.

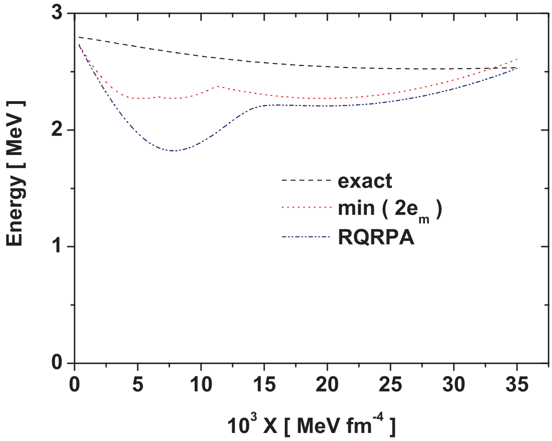

Fig. 6. The first excited state energies predicted by the renormalized QRPA are compared with the energy of the first 2^+ state, given by the exact calculation in the case of four nucleons moving in the single shell $j = 13/2$. The minimal two quasiparticle energies are also presented. The three sets of energies are plotted as function of the QQ interaction strength, X. The RQRPA results correspond to $q_0 = 40\,\text{fm}^2$.

be extended also to the realistic multi-shell case. Having this in mind, we compare the results obtained with our method with the exact ones in Figs. 5 and 6. To simplify the calculations, we consider the cases of two and four particles in the shell $i_{13/2}$ correlated with pairing, of strength $G = 0.4\,\text{MeV}$, and the long QQ interaction. Details about the exact calculations can be found in Refs. 33–36. As shown in Fig. 5, the exact result for two particles exhibits a linear dependence on

X. The linear dependence on X is determined by the fact that the $J = 2$ matrix elements of the QQ interaction are linear function of X and moreover, they do not feel the pairing force. The RQRPA result depends on the magnitude of q_0, involved in the restriction concerning the average value of the quadrupole moment. We fixed q_0 such that the energies of the first excited state predicted by the RQRPA and exact calculations are close to each other, at the end of the considered interval. The two energies are close to each other also for small values of X. The largest deviation from the exact result, about 1 MeV, is met for that strength X, where the RQRPA excitation energy is minimum. After reaching the minimum value, the energy of the first excited state is increasing with X, passes through a maximum, at $X \approx 15 \cdot 10^{-3}\,\mathrm{MeV\,fm^{-4}}$, then slowly decreases, exhibits a flat minimum at $X \approx 23 \cdot 10^{-3}\,\mathrm{MeV\,fm^{-4}}$ and then continuously increases.

The case of four particles exhibits a more complex structure. The exact energy is a decreasing function of X, meets a flat minimum and then slowly increases. The largest deviation of the RQRPA result from the exact one is about 1 MeV but in most of the considered interval the deviation keeps with 500 keV. Note that, in both cases of two and four particles the exact result is closer to the minimal 2 quasiparticle energies than to the RQRPA result. That means that the RQRPA overestimate the state collectivity. The curves of 2qp and RQRPA energies look similarly with those corresponding to two particles calculations.

It seems that the agreement between the RQRPA and exact results is better for larger number of particles. We explain this feature in the following manner. The QQ interaction has a contribution not only in the ph channel but also in the *pp* channel. The contribution in the *pp* channel is negligible small for a large number of particles but important for a low particle number. The contribution in both channels is fully taken into account by the exact method. Although our procedure, to some extent, includes both effects it seems that for a small number of particles a good portion of the *pp* contribution is lost. Since the long range interaction in the *pp* channel is repulsive, it is obvious that adding the missing terms the energy would increase and consequently the agreement with the exact result is substantially improved.

Note that the final results in the present approach are obtained with a succession of three approximations, two BCS-like and one of QRPA type. Since one cannot separate the effects of each of the three approximations, the deviation from the exact result could not be attributed separately to each of the three approaches. Moreover, while the exact calculation yields states of good angular momentum the second-order BCS and RQRPA states are deformed. Therefore, the comparison between the two procedures assumes that the angular momentum of the state predicted by the exact calculation is the dominant component of the RQRPA state.

Having these features in mind, a more fair comparison would be between the standard and renormalized QRPA. One notices that the RQRPA extends the QRPA beyond the critical value of the QQ strength where the standard QRPA breaks down. The RQRPA takes into account all terms of the quasiparticle Hamiltonian which are ignored by the standard QRPA. This is possible due to the BCS treatment of the quadrupole pairing correlations. A similar effect is induced in Ref. 29 by the *attached* field. Although the standard QRPA includes the QQ interaction, the resulting states have the angular momentum and its projection on the z-axis as good quantum numbers. By contrast, here the RQRPA states are deformed for any interaction strength. While in the standard QRPA, starting from the critical interaction strength the single particle basis should be deformed, here both spherical and deformed nuclei are described in an unified fashion with a sole single particle basis. As mentioned in introduction, several authors used deformed QRPA methods. Without exception they use a deformed single particle mean field or a consistent deformed HFB + QRPA. Here, the starting single particle basis is spherical and deformation is induced at the quasiparticle representation level. A procedure similar to that presented here was used to study the double beta Fermi transition.[32] In the quoted paper, after the first BV transformation for nucleons of similar charge the two body interaction describes the proton–neutron quasiparticle pairing interaction. Therefore, the second BV transformation mixes protons with neutrons. The first root of the pnQRPA approach for the newly defined quasiparticles, represented as function of the attractive interaction strength looks similarly with the harmonic energy dependence on the QQ interaction strength, described in this paper. As shown by Fig. 8 of the mentioned reference, the proposed formalism approximates very well the exact result obtained through diagonalization.

For the sake of simplicity, the proposed method was applied to the case of a separable two body interaction but can be used for any interaction as well. In particular, that is also true for Skyrme or Gogny HFB+QRPA approaches without much computational efforts.

5. Comparison with the HFB Formalism

The HFB approach is based on defining a set of quasiparticle operators as being a generalized unitary and linear transformation of the creation and annihilation operators of particles in spherical shell model states.[37] The vacuum state for such operators is a function $|\Phi\rangle$ depending on the transformation coefficients, which are to be determined variationally, in order to describe the ground state. Applying the HFB transformation to the many body Hamiltonian with paring + quadrupole interaction (2.1), one obtains the single particle Hamiltonian

$$H_{\mathrm{HFB}} = \sum_{\alpha}(\epsilon_a - \lambda)c^{\dagger}_{\alpha}c_{\alpha} - \frac{1}{4}\sum_{\mu=-2}^{2} q_{\mu}(Q_{\mu} + Q^{+}_{\mu}) - \frac{1}{4}p_0(P + P^{+}), \quad \text{with} \tag{4.16}$$

$$q_{\mu} = \frac{X}{2}\langle\Phi|Q_{\mu}|\Phi\rangle, \quad p_0 = \frac{G}{2}\langle\Phi|Q_{\mu}|\Phi\rangle, \tag{4.17}$$

where we assumed that q_{μ} and p_0 are real numbers. According to the Bloch–Messiah theorem,[38] the unitary HFB transformation can be written as a product of three successive transformations. The first transformation is of a Hartree–Fock type, performed within a canonical single particle basis defined by diagonalizing the Nilsson Hamiltonian

$$h = \sum_{\alpha} (\epsilon_a - \lambda) - \frac{1}{2} q_0 Q_0 - \frac{1}{2} q_2 (Q_2 + Q_{-2}). \tag{4.18}$$

The second factor is a BV transformation, depending on the occupation probabilities v_i^2, with the gap parameter $\Delta = p_0$. By this transformation, one distinguishes between the "paired" levels and "blocked" levels, which could be either occupied ($v_i = 1; u_i = 0$) or empty ($v_i = 0; u_i = 1$). Further, the newly defined quasiparticles are linearly transformed with a Hartree–Fock like transformation, determined such that the total energy

$$E(q_0, q_2, \Delta) = \langle \Phi | H | \Phi \rangle = \sum_i \widetilde{\epsilon}_i v_i^2 + \frac{1}{X}(q_0^2 + q_2^2) - \frac{\Delta^2}{G} \tag{4.19}$$

is minimized. Here $\widetilde{\epsilon}_i$ denotes the energy of the Nilsson state $|i\rangle$. Equations (4.19) and (4.17) are to be simultaneously solved, by an iterative procedure. The small oscillations around the stationary values of the deformation q_0, q_2 and the gap energy Δ, corresponding to the minimum energy, are described by the QRPA equations.

Let us now enumerate the differences between our approach and the HFB method. By contrast to the HFB approach, which consists of a product of two Hartree–Fock and one Bogoliubov transformation, in our case the transformation of the spherical single particle basis is a product of two Bogoliubov type transformations. While the first factor is a standard Bogoliubov transformation, which preserves the rotation symmetry, the second one mixes the quasiparticles and quasiholes and moreover the coefficients depend on the magnetic quantum number. Therefore, the new quasiparticles are deformed. While the first Bogoliubov transformation treats the spherical mean field and the pairing, the second transformation accounts for a piece of the QQ interaction.

It is well-known, that for treating the collective motion of a many body system, it is very important to choose the optimal single particle basis. If the nucleus under consideration is only weakly deformed or spherical, the pairing interaction dominates and defines the quasiparticle representation, the long range interaction being treated at the QRPA level. When the nucleus is well deformed, the long range interaction is treated first, i.e., a deformed single particle basis is defined, and then the pairing correlation are switched on. The new representation is used within the QRPA formalism to determine the collective effects.

We note that our procedure achieves a compromise of the two paths. The deformation is, indeed, taken into consideration in the quasiparticle representation and afterwards the residual interaction is treated by the QRPA. The Nilsson states defined within the HFB approach, do not have j as good quantum number, while the deformed quasiparticles used in the present work have a definite j, which reflects the fact that deforming the quasiparticles only a small part of the quadrupole interaction is involved. As a matter of fact that picture might be a good approximation for small nuclear deformation. Actually, the main effect of the QQ interaction is introduced as the QRPA effect. Here, the deformed quasiparticle energies depend linearly on the deformation despite the complex deformation dependence of the composing terms $\bar{E}_\alpha$ and δ_α. This is again due to the small magnitude of the nuclear deformation.

There are some differences between our approach and the HFB when the QRPA is defined. In the case of HFB the first QRPA energy is a decreasing function of the nuclear deformation. Therefore, in the region of level crossing, the minimal two quasiparticle energies are very small and one expects that the approximation collapses. Of course, such a situation does not show up in our case due to the quasiparticle energy dependence on the deformation. The QRPA, built on the top of the HFB ground state, takes into account only the quasiparticle long range correlations due to the bi-quasiparticle operators and their Hermitian conjugate. By contrast, as we have already mentioned, the RQRPA described here includes also the quasiparticle density operators. The first energy solution of the RQRPA equations does not collapse irrespective the magnitude of the long range interaction strength. Moreover, beyond the strength where the first excitation energy reaches a minimum value, this is an increasing function of X. This reflects the fact that beyond the critical strength the repulsive component of the long range interaction in the deformed quasiparticle representation, prevails over the attractive one.

6. Summary and Conclusions

In the previous sections, we formulated an approach of renormalizing the QRPA such that no breaking down shows up. Indeed, the first QRPA energy, instead of vanishing, it becomes minimum and then, by increasing the long range interaction strength, is increasing. Things happen as if the effective interaction changes its character, from attractive to an repulsive one. The formalism redefines first the system ground state by accounting for the quasiparticle quadrupole pairing interaction. Moreover, on the top of the newly defined ground state a QRPA description is constructed. It turns out that the drawback of the standard QRPA of collapsing for a critical value of the interaction strength, is removed. In the new picture some higher QRPA dynamics is included. Indeed, the scattering terms are effectively participating in building up the new phonon operator.

We note that the new quasiparticles are not tensors of definite rank and projection. They have however, a definite j. This makes the difference with the picture where first one defines a deformed mean field and then the pairing correlations are considered. In this case j is not a good quantum number, but Ω is. This difference favors the present approach, when the QRPA is supplemented by an angular momentum projection operation of the many body states.

The states considered in the present work are characterized by $K = 0$ and therefore by the total angular momentum projection, finite bands of $K = 0$ can be defined.

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