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A complex integration technique to remove spurious states associated with spontaneously broken symmetries in RPA calculations

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Abstract

The removal of the spurious states associated with the violation of rotational and gauge invariance by mean field approximation from the RPA solutions describing the low-energy spectrum of nuclei is a notoriously difficult task, in particular in a rotating frame. A novel, numerically accurate yet technically simple method to accomplish this aim has been developed based on linear response theory. The results of calculations carried out for the deformed, superfluid, rotating nucleus ^{168}Yb testify to the power of the technique, the associated solutions respecting the variety of sum rules required to be fulfilled by the RPA solutions because of conservation laws.

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1. Introduction

A very useful approach to the nuclear many-body problem is the mean field approximation. As a rule, mean field solutions violate a number of symmetries, in particular

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rotational invariance (Nilsson model) and gauge invariance (non-conservation of particle number associated with the BCS Hamiltonian) (cf. e.g. Refs. [1–7])). Furthermore, the mean field potential violates translational symmetry.

The restoration of the invariance of the total Hamiltonian can be accomplished by including the effects of a collective field generated by a small rotation (in 3D or in gauge space) or a displacement of the system as a whole [1]. The spectrum of the normal modes generated by the resulting particle-field coupling, treated e.g. in the random phase approximation (RPA), contains an excitation mode with zero-frequency, ensuring that all finite energy excitations of the system are "orthogonal" to the "spurious" degree of freedom associated with the broken symmetry.

The presence of a zero-frequency mode, and the related rotational bands in 3D and in gauge space (quadrupole rotational [1] and pairing rotational bands [8] experimentally observed in inelastic [9] and two-particle transfer processes respectively [10]) are a manifestation of a general theorem [11] which states that the spontaneous breaking of a continuous symmetry leads to a new branch of the excitation spectrum, the Nambu–Goldstone mode, which has zero energy.

To the extent that one calculates the RPA solutions of the particle-field coupling with self-consistent single-particle energies and wavefunctions, the "spurious" excitations have exactly zero excitation energy and are completely orthogonal to the physical excitations (e.g. β- and γ-vibrations in a deformed nucleus). In actual calculations, the RPA treatment of the particle-field coupling may fail to restore the original symmetry of the Hamiltonian for a number of reasons such as the use of non-self-consistent single-particle energies and wavefunctions, truncation of the configuration space, etc. In any case, the exact separation of spurious states is a necessary condition to be fulfilled by any theoretical treatment.

A variety of methods explaining how to treat spurious states [6,7,12] have been proposed in literature. We have found them, however, not useful to deal with our specific problem, where the so-called RPA response functions (polarization propagators) are used in place of solving the RPA eigenvalue equation searching for every single root. In fact, because of the high density of the particle–hole spectrum in deformed, rotating nuclei, the RPA solutions needed, for example, in the calculations of the ground state correlation energy [13] or the single-particle self-energy [14], are to be calculated in a coarse mesh approximation, like the one provided by linear response theory. While in the "discrete" solution of the RPA equations, where every single root is calculated, the search for the spurious ($\omega = 0$) state is straightforward, this is not the case within the framework of a coarse grain approximation. To overcome this limitation of linear response theory with broken symmetries, we have developed a technique which makes it possible to remove the spurious contribution of the broken symmetry phenomena from the RPA response function without modifying the original Hamiltonian.

The paper is organized in the following way: Section 2 is devoted to introduce the RPA response function. In Section 3 we will explain the method to evaluate and remove the spurious contributions when their energies are real. In Section 4 we will show that this method can be used to calculate sum rules also. In Section 5 we generalize

the method when the spurious states have purely imaginary energies while Section 6 contains applications of this new technique to the case of a well-deformed nucleus, that is ^{168}Yb. Section 7 is devoted to the conclusion.

2. The RPA response function

In this section we follow mainly the notation of the general formulation of RPA response function given in Ref. [15]. The starting point of the calculation is the resolvent operator $\hat{G}(\omega) \equiv (\hat{H} - \omega)^{-1}$. The response function for general hermitian one-body operators $\hat{C}$ and $\hat{D}$ is given by

$$\mathcal{R}_{CD}(\omega) \equiv C^{\dagger} G(\omega) D, \tag{1}$$

where $G(\omega)$ is the matrix corresponding to the resolvent operator $\hat{G}(\omega)$, and C and D are column vectors representing the RPA part of one-body operators $\hat{C}$ and $\hat{D}$. The matrix, $G(\omega)$, can be calculated once the RPA eigenvalue problem is solved, that is

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \omega_n \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix}. \tag{2}$$

One has to take into account that there are two different kinds of RPA eigenvalues, the non-zero energy solutions corresponding to intrinsic excitations as β- and γ-vibrations and the zero-energy solutions related to the breakdown of a symmetry. The matrix $G(\omega)$ and, as we will see below the response function, is then the sum of two terms $G^{\mathrm{exc}}(\omega)$ and $G^{\mathrm{NG}}(\omega)$ describing, respectively, physical excitations and spurious states (zero-energy modes).

In fact, for non-zero real solutions, the eigenvalues and eigenvectors of Eq. (2) appear in doublets: $\big((\omega_n, Z_n), (-\omega_n, \bar{Z}_n)\big)$, where the eigenvectors $Z_n, \bar{Z}_n$ are defined as

$$Z_n = \begin{pmatrix} X_n \\ Y_n \end{pmatrix} \leftrightarrow \hat{Z}_n^{\dagger} = \sum_{\alpha<\beta} \left[X_n(\alpha\beta) a_\alpha^{\dagger} a_\beta^{\dagger} + Y_n(\alpha\beta) a_\beta a_\alpha \right], \tag{3}$$

$$\bar{Z}_n = \begin{pmatrix} Y_n^* \\ X_n^* \end{pmatrix} \leftrightarrow \hat{Z}_n = \sum_{\alpha<\beta} \left[Y_n^*(\alpha\beta) a_\alpha^{\dagger} a_\beta^{\dagger} + X_n^*(\alpha\beta) a_\beta a_\alpha \right]. \tag{4}$$

In the notation above we have used the equivalence of the RPA part of an arbitrary one-body operator $\hat{Z}_n^{\dagger}$ with a column vector Z_n. In this particular case, $\hat{Z}_n^{\dagger}$ is the creation operator of the RPA eigenmode corresponding to the excited states $|n\rangle$, and the normalization condition is

$$[\hat{Z}_n, \hat{Z}_{n'}^{\dagger}]_{\mathrm{RPA}} = \delta_{nn'}, \tag{5}$$

where the commutator between two operators within the harmonic approximation results in a c-number and is defined by an inner product of the corresponding vectors,

$$[\hat{C}^{\dagger}, \hat{D}]_{\mathrm{RPA}} = C^{\dagger} I D, \qquad I = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{6}$$

The resolvent matrix can then be written in terms of these solutions as

$$G^{\mathrm{exc}}(\omega) = \sum_n \left[\frac{Z_n * Z_n^\dagger}{\omega_n - \omega} + \frac{\bar{Z}_n * \bar{Z}_n^\dagger}{\omega_n + \omega} \right], \tag{7}$$

where $Z_1 * Z_2^\dagger$ represents a matrix constructed from the two vectors Z_1 and Z_2 according to the relation

$$C^\dagger (Z_1 * Z_2^\dagger) D = [\hat{C}^\dagger, \hat{Z}_1^\dagger]_{\mathrm{RPA}} [\hat{Z}_2, \hat{D}]_{\mathrm{RPA}}, \tag{8}$$

for arbitrary one-body operators $\hat{C}$ and $\hat{D}$. We define the transition matrix elements between an RPA excited state $|n\rangle$ and the ground state $|0\rangle$ as $\mathcal{Q}_C(n) \equiv \langle n|\hat{C}|0\rangle = [\hat{Z}_n, \hat{C}]_{\mathrm{RPA}} = Z_n^\dagger I C$.

The response function for one-body hermitian operators $\hat{C}$ and $\hat{D}$ in the RPA scheme for non-zero real solutions is given by

$$\begin{aligned} \mathcal{R}_{CD}^{\mathrm{exc}} &= \sum_n \left\{ \frac{C^\dagger (Z_n * Z_n^\dagger) D}{\omega_n - \omega} + \frac{C^\dagger (\bar{Z}_n * \bar{Z}_n^\dagger) D}{\omega_n + \omega} \right\} \\ &= \sum_n \left\{ \frac{\mathcal{Q}_C^*(n) \mathcal{Q}_D(n)}{\omega_n - \omega} + \frac{\mathcal{Q}_C(n) \mathcal{Q}_D^*(n)}{\omega_n + \omega} \right\}. \end{aligned} \tag{9}$$

For zero-energy solutions, the eigenvalues of the RPA equation (see Eq. (2)) are twofold degenerate [3,4,6,16]. Accordingly, there are two vectors (P_a, Q_a) of the form

$$P_a = \begin{pmatrix} p_a \\ p_a^* \end{pmatrix}, \qquad Q_a = \begin{pmatrix} q_a \\ -q_a^* \end{pmatrix}, \tag{10}$$

satisfying the equation $[\hat{H}, \hat{Q}_a]_{\mathrm{RPA}} = \hat{P}_a$. Note that $\hat{P}_a^\dagger = \hat{P}_a$ and $\hat{Q}_a^\dagger = -\hat{Q}_a$. In the above relation, $\hat{P}$ generates the collective operation needed in restoring the symmetry of the original Hamiltonian, that is linear momentum $\hat{P}$ in the case of translational invariance, angular momentum $\hat{J}$ in the case of rotational invariance and particle number $\hat{N}$ in the case of gauge invariance. The moment of inertia tensor g_{ab} associated with the corresponding collective modes (translation, and rotation in 3D and gauge space) can be calculated in terms of the operators $\hat{P}$ and $\hat{Q}$ according to $g_{ab} \equiv [\hat{P}_a^\dagger, \hat{Q}_b]_{\mathrm{RPA}}$. It is then possible to calculate the so-called "angle" operator canonical conjugate to $\hat{P}_a$ as $-i\hbar \sum_b (g^{-1})_{ab} \hat{Q}_b$. The possibility that there are more than one spurious mode is reflected by the presence of the indices a and b. Using these definitions one can write the matrix resolvent for the zero-energy solutions as

$$G^{\mathrm{NG}}(\omega) = \sum_{a,b} (g^{-1})_{ab} \left[\frac{P_a * P_b^\dagger}{-\omega^2} + \frac{Q_a * P_b^\dagger + P_a * Q_b^\dagger}{-\omega} \right]. \tag{11}$$

The corresponding RPA response function can then be written as

$$\mathcal{R}_{CD}^{\mathrm{NG}} = \sum_{a,b} (g^{-1})_{ab} \left\{ \frac{[\hat{C}^\dagger, \hat{P}_a][\hat{P}_b, \hat{D}]}{-\omega^2} + \frac{[\hat{C}^\dagger, \hat{Q}_a][\hat{P}_b, \hat{D}] - [\hat{C}^\dagger, \hat{P}_a][\hat{Q}_b, \hat{D}]}{\omega} \right\}, \tag{12}$$

where we have neglected the subscript RPA in the commutators, for simplicity. From the equation above one can see that, if one deals with operators which satisfy $[\hat{C},\hat{P}]_{\rm RPA} = [\hat{D},\hat{P}]_{\rm RPA} = 0$, then the corresponding spurious state contribution to the response function $\mathcal{R}^{\rm NG}_{CD}$ is zero. However, if one takes into account an operator $\hat{C}$ or $\hat{D}$ which does not commute with the generator of the collective mode restoring the broken symmetry $\hat{P}$, this leads to a quadratical divergence in the $\mathcal{R}^{\rm NG}$ response when $\omega \to 0$. This can happen when one considers $\hat{C} = \hat{D} = \hat{Q}_{21}$ (where $\hat{Q}_{21}$ is a component of the multipole operator $\hat{Q}_{\lambda\mu}$) and $\hat{P} = \hat{J}_x$, that is the operator that restores the rotational invariance. The same situation appears with the pairing operators $\hat{P}_\tau(\tau = n,p)$ which do not commute with the particle number operator $\hat{N}$ (gauge invariance). Consequently, one is confronted with the problem of eliminating the contribution of $\mathcal{R}^{\rm NG}_{CD}(\omega)$ from the total RPA response function. In fact, the RPA equation (the Dyson equation) can be solved through $\hat{G}(\omega) = (1 + \hat{G}_0(\omega)\hat{V})^{-1}\hat{G}_0(\omega)$, where $\hat{G}_0(\omega)$ is the resolvent operator of the unperturbed Hamiltonian $\hat{H}_0$, while $\hat{V}$ is the residual interaction leading to the total Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$. One has to remember that $\hat{G}(\omega) = \hat{G}^{\rm exc}(\omega) + \hat{G}^{\rm NG}(\omega)$ so that the resultant response function $\mathcal{R}_{CD}(\omega)$ includes contributions of the spurious modes (see Eq. (1)). The physically relevant part containing only the real excitations of the system is thus $\mathcal{R}^{\rm exc}_{CD} = \mathcal{R}_{CD}(\omega) - \mathcal{R}^{\rm NG}_{CD}(\omega)$.

In the following we describe how to evaluate the spurious contribution $\mathcal{R}^{\rm NG}_{CD}(\omega)$ and to subtract it from the total RPA response either when the energies of the spurious modes are real or purely imaginary, the two cases of actual interest in connection with the RPA solutions (see Eq. (2)). It is worthwhile noticing that the method also provides an alternative way to calculate each RPA root and associated strengths of arbitrary operators, although it is particularly efficient in dealing with the spurious mode problem.

3. Removal of the "real" spurious modes

Our problem is how to calculate $\mathcal{R}^{\rm NG}_{CD}(\omega)$. If the spurious modes are exactly decoupled to zero energy, $[\hat{H},\hat{P}_a] = 0$, then it is enough to calculate $\mathcal{R}^{\rm NG}_{CD}(\omega)$ according to Eq. (12). However, some approximations are inevitable in actual calculations, which shift the energies of the spurious states away from zero by an unknown amount. The elimination of this contribution is, in principle, straightforward if one can obtain the wavefunctions of the RPA eigenmodes corresponding to the shifted spurious modes, $\omega_{\rm NG} \approx 0$, as defined in Eqs. (2) and (3). This is, however, a numerically subtle problem because the associated contributions diverge very rapidly as $\omega \to 0$ (cf. Eq. (12)). It is more convenient to work out the RPA response directly. We shall, in what follows, show how this can be done. The underlying idea is based on Cauchy's integral formula, namely the integration of an analytic function on a closed contour where the function is bounded. This theorem states that the evaluation of contour integrals is equivalent to the algebraic computation of residues at singular points, that is

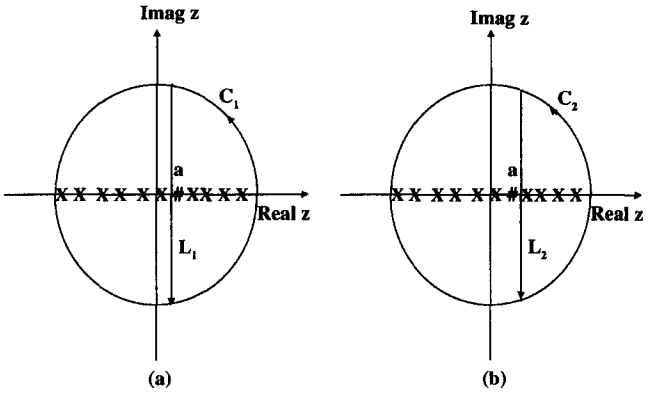

Fig. 1. Real poles of a generic function $f(z)$. (a) The contour encircles the unknown pole a. (b) The contour does not encircle the pole a.

$$\oint_C \frac{dz}{2\pi i} f(z) = \sum_i \mathrm{Res}_i, \tag{13}$$

where the integration path C is chosen in such a way that all poles of the function $f(z)$ lie inside the contour of integration and the notation Res_i means the residue of the function $f(z)$ corresponding to the pole i. The equality above can be applied directly if one knows all poles and residues of the function $f(z)$ taken into account. However, because $f(z) = -\mathcal{R}_{CD}(z)$, one needs to obtain the amplitudes, $\mathcal{Q}_C^*(n)\mathcal{Q}_D(n)$, and the eigenenergies, ω_n, corresponding to the spurious states which are unknown due to their shift away from zero. Therefore, we need to calculate numerically the complex integral appearing on the left-hand side of Eq. (13). The energies of the spurious modes are the poles of the response function (see Eq. (9)) while the amplitudes $\mathcal{Q}_C^*(n)\mathcal{Q}_D(n)$ are the corresponding residues.

In what follows we assume that $f(z)$ is an analytic function with real poles (see Fig. 1). Our aim is to evaluate one of the poles (marked with # in Fig. 1 and labeled with the letter a) and its residue without knowledge of the value of the pole. To achieve this goal one can apply Cauchy's theorem twice, using two different contours which include or leave out, respectively, the contribution of the singularity at a. One can choose different paths of integration that lead to the same result. A convenient contour of integration is the one indicated in Fig. 1.

We start considering the path $D_1 = C_1 + L_1$ that encircles the pole a (see Fig. 1a). The result of the integration along this path is

$$\oint_{D_1} \frac{dz}{2\pi i} f(z) = \sum_{r_+} \mathrm{Res}_{r_+}, \tag{14}$$

where r_+ means sum over positive poles on the real axis included by D_1. We consider now a second contour indicated by $D_2 = C_2 + L_2$ (see Fig. 1b), that excludes the pole a. Cauchy's theorem gives

$$\oint_{D_2} \frac{dz}{2\pi i} f(z) = \sum_{r_+} \mathrm{Res}_{r_+} - \mathrm{Res}_a. \tag{15}$$

Subtracting the result of these integrations, one obtain the residue Res_a without knowing the exact value of the pole a. Now one has to find an equivalent expression that can be used to calculate the pole itself. For this purpose, we introduce other integrals of functions $f(z)/z^n$ $(n \geqslant 1)$, which have the same singularities as those of $f(z)$ plus the additional pole at $z = 0$, i.e.

$$I_n(a) = \oint_{D_1} \frac{dz}{2\pi i} \frac{f(z)}{z^n} - \oint_{D_2} \frac{dz}{2\pi i} \frac{f(z)}{z^n} \quad (n \geqslant 0). \tag{16}$$

One should note that the case $n = 0$ was already taken into account in Eqs. (14) and 15) and that, due to the fact that the chosen paths do not encircle zero, the singularities contributing to the integrals of Eq. (16) for all functions $f(z)/z^n (n \geqslant 0)$ are the same. Using these considerations, we can write that

$$I_n(a) = \frac{\mathrm{Res}_a}{a^n} \quad (n \geqslant 0). \tag{17}$$

At this point we can combine the results with $n = 0$ and $n = 1$, getting $a = I_0(a)/I_1(a)$, that is the value of the unknown pole.

After transforming the complex integration $I_n(a)$ into real variable integration and taking the limit of infinite radius of the circle in Fig. 1, we can summarize all steps of our technique as

$$\begin{aligned}
&\text{step 1} \longrightarrow \text{evaluate} \quad I_0(a) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \left[f(i\omega + b_2) - f(i\omega + b_1) \right], \\
&\text{step 2} \longrightarrow \text{evaluate } I_1(a) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \left[\frac{f(i\omega + b_2)}{i\omega + b_2} - \frac{f(i\omega + b_1)}{i\omega + b_1} \right], \\
&\text{step 3} \longrightarrow \text{obtain } a = \frac{I_0(a)}{I_1(a)},
\end{aligned} \tag{18}$$

where b_1 and b_2 are the positions of the vertical straight line L_1 and L_2 of the chosen paths with the condition $b_1 < a < b_2$. With the pole and it's residue we can reconstruct the contribution of the spurious mode $\omega_{\mathrm{NG}} = a$.

As seen from Eq. (18) and Fig. 1, the success of the method is based on the proper choice of the b-values, i.e. the interval (b_1, b_2) which contains only the pole under study. In order to confirm that only one pole is inside the interval the following procedure should be added:

$$\text{step 4} \longrightarrow \text{check} \quad \frac{I_0(a)}{I_2(a)} = \left(\frac{I_0(a)}{I_1(a)} \right)^2. \tag{19}$$

If the equality in step 4 is not satisfied, the interval should be shrunk until the relation defined in Eq. (19) holds. This is not a difficult task in our calculations because the spurious modes (our unknown poles) lie very close to zero (as we have explained in the introduction). We will show below in the case of ^{168}Yb how it is possible to accurately fix the interval (b_1, b_2).

4. Sum rules in integral form

Before analyzing the case of spurious states with imaginary energy, we want to show that the contour integration is an alternative method to calculate sum rules, useful yardsticks for quantitatively measuring the degree of collectiveness of a given state [1–4] but, above all, within the present context, expression of very general relations between operators reflecting basic conservation rules, to be fulfilled by theory, in particular RPA theory.

Let us assume that $\hat{F}$ is a generic one-body hermitian operator. We define as sum rule the quantity

$$S_k(F) \equiv \sum_n (E_n - E_0)^k |\langle n|\hat{F}|0\rangle|^2 = \sum_n \omega_n^k |\langle n|\hat{F}|0\rangle|^2, \tag{20}$$

which represents the kth moment of the distribution of the excitation strength $|\langle n|\hat{F}|0\rangle|^2$ produced by the operator $\hat{F}$ and where n indicates an excited state with energy ω_n. The expression above is straightforward to evaluate but for doing so one needs to have a detailed knowledge of each single excited states n. This requirement can be circumvented using the RPA response function and contour integration for the moments with $k \leqslant 0$.

The following description is based on the spectral representation of the linear response given in Eq. (9), which has the advantage of displaying explicitly the corresponding analytic properties, namely poles at $+\omega_n$ and $-\omega_n$ with residues $-\mathcal{Q}_F^*(n)\mathcal{Q}_F(n)$ and $\mathcal{Q}_F(n)\mathcal{Q}_F^*(n)$, respectively. At this point we can apply the Cauchy's integral formula for the analytic function, $\mathcal{R}_{FF}(z)/z^{-k}$, with a contour shown in Fig. 1a, to calculate the kth moment, obtaining

$$S_k(F) = \sum_n \omega_n^k \mathcal{Q}_F(n)\mathcal{Q}_F^*(n) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \mathrm{Re}\left[\frac{\mathcal{R}_{FF}(i\omega + b_1)}{(i\omega + b_1)^{-k}}\right] \quad (k \leqslant 0). \tag{21}$$

In working out this result we have used the fact that $\mathcal{R}_{FF}(z) \sim 0(1/z^2)$ as $z \to \infty$ for the "diagonal response", so that the contribution from the semicircle C_1 in Fig. 1a vanishes as long as $k \leqslant 0$. Note that the $k = 0$ moment, called, the *non-energy weighted sum rule* (NEWSR), corresponds to the sum of all transition matrix elements between excited states and the ground state. The $k = -1$ moment is called the *inverse energy weighted sum rule* (IEWSR), which is related to the polarizability of the system with respect to an external field given by the operator $\hat{F}$. The parameter b_1 is chosen in such

a way that all the positive real RPA solutions are encircled by the chosen path, that is $0 < b_1 < \omega_1$ where ω_1 is the lowest RPA root.

We want to stress that there is the possibility to check this integration method in the case of the IEWSR, because one can evaluate this sum rule by a simple relation [3],

$$\sum_n \frac{\mathcal{Q}_F(n)\mathcal{Q}_F^*(n)}{\omega_n} = \tfrac{1}{2}\,\mathrm{Re}\,[\mathcal{R}_{FF}(\omega = 0)]\,. \tag{22}$$

Note that if the spurious modes have real energies this expression includes their (divergent) contributions in both sides, which should be eliminated by the method explained in the previous section.

5. Removal of "imaginary" spurious modes

The scenario depicted above is valid only when the energies of these spurious contributions are real. We have found that, at finite rotational frequency, the spurious modes can have purely imaginary energies. This should not be surprising because the RPA equation itself, can have non-zero complex solutions (cf. Eq. (2)). If the symmetry conserving Hamiltonian is treated exactly, the appearance of imaginary solutions represents instabilities of the system. It is, however, noted that approximate treatments of the self-consistent problem, as those already mentioned in the introduction, may lead to a shift of the energy of the spurious states to imaginary values.

Let us restrict the discussion to the case in which the matrix elements of the Hamiltonian are real (cf. Ref. [15] for a discussion of the more general situation). The imaginary root appears in doublets in a different form as that appearing in the case of real roots: $\{(\omega_m, Z_m), (-\omega_m = \omega_m^*, Z'_m)\}$, where

$$Z'_m = \begin{pmatrix} X_m^* \\ Y_m^* \end{pmatrix} \leftrightarrow \hat{Z}'^{\dagger}_m = \sum_{\alpha<\beta} \left[X_m^*(\alpha\beta) a_\alpha^\dagger a_\beta^\dagger + Y_m^*(\alpha\beta) a_\beta a_\alpha \right]. \tag{23}$$

While the notation used here is similar to that used in the case of real roots (see Section 2), one has to pay attention to the different definition of the RPA creation operator $\hat{Z}_m$ in the case of purely imaginary solution ω_m. $\hat{Z}_m$ is related to the corresponding operator for real solution by a complex conjugation changing the nature of the transition matrix elements $\mathcal{Q}_C^*(m)\mathcal{Q}'_D(m)$, which are the residues of the imaginary pole ω_m.

One can notice that $[\hat{Z}_m, \hat{Z}^\dagger_{m'}]_{\mathrm{RPA}} = 0$ and the normalization condition is now

$$[\hat{Z}_m, \hat{Z}'^{\dagger}_{m'}]_{\mathrm{RPA}} = \delta_{mm'}. \tag{24}$$

Accordingly, the contributions of the imaginary roots to the resolvent matrix takes different form from those shown in Eq. (7);

$$G^{\mathrm{IM}}(\omega) = \sum_m \left[\frac{Z_m * Z_m'^{\dagger}}{\omega_m - \omega} + \frac{Z'_m * Z_m^{\dagger}}{\omega_m + \omega} \right], \tag{25}$$

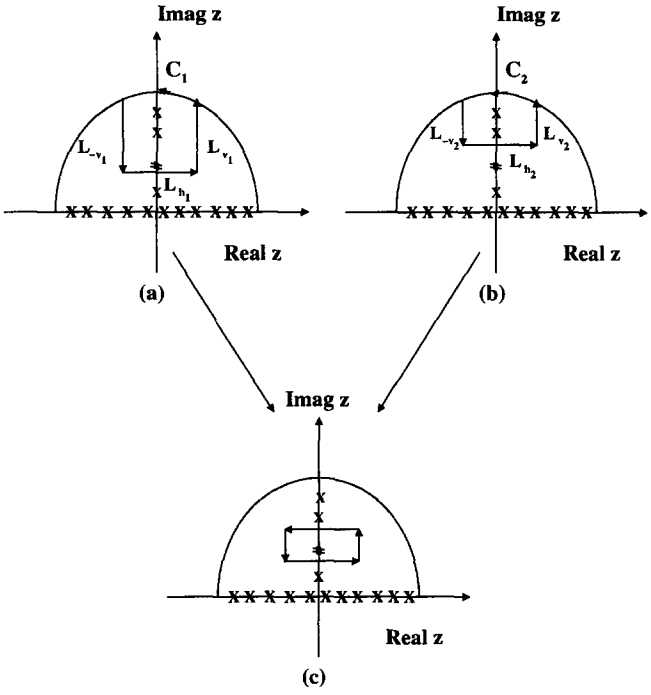

Fig. 2. Imaginary poles of a generic function $f(z)$. (a) The contour encircles the unknown pole a. (b) The contour does not encircle the pole a. (c) Difference between path (a) and (b).

where the summation is taken with respect to the imaginary roots, and so does the contributions to the response function:

$$\mathcal{R}_{CD}^{\mathrm{IM}} = \sum_m \left\{ \frac{\mathcal{Q}_C^*(m)\mathcal{Q}'_D(m)}{\omega_m - \omega} + \frac{\mathcal{Q}'_C(m)\mathcal{Q}_D^*(m)}{\omega_m + \omega} \right\}. \tag{26}$$

The basic strategy is the same as in the case of real spurious modes. However, the contour of integration explained before is not applicable in the present situation. As done before, we start with a generic function $f(z)$ with two different kinds of poles, real and purely imaginary (Fig. 2).

Using Cauchy's theorem one can write

$$\oint_{D_1} \frac{dz}{2\pi i} f(z) = \sum_{i_+} \mathrm{Res}_{i_+}, \tag{27}$$

where $\sum_{i_+}$ means positive imaginary poles contained in the contour path $D_1 = C_1 + L_{v1} + L_{-v1} + L_{h1}$ (see Fig. 2). To evaluate the pole marked with a one needs to proceed in the same way as explained in Section 3, but choosing paths on the upper half part of the complex plane. Choosing a second path $D_2 = C_2 + L_{v2} + L_{-v2} + L_{h2}$ that does not contain the imaginary pole, one can write, in analogy to the real case

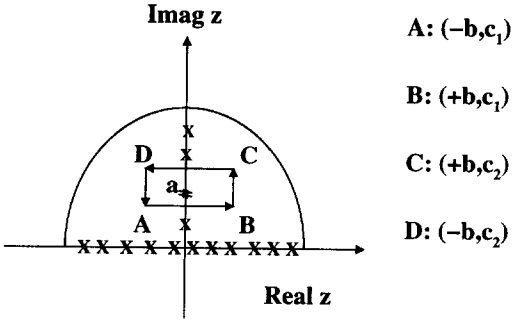

Fig. 3. Contour integration for an imaginary pole in terms of a real variable.

$$I_n(a) = \oint_{D_1} \frac{dz}{2\pi i} \frac{f(z)}{z^n} - \oint_{D_2} \frac{dz}{2\pi i} \frac{f(z)}{z^n} = \frac{\mathrm{Res}_a}{a^n} \quad (n \geqslant 0). \tag{28}$$

In this particular case, all the calculations can be greatly simplified if we move only the horizontal lines when choosing the contour paths. This implies that the two arcs C_1 and C_2 actually coincide and the difference between the contours transforms in a rectangular contour integration encircling the pole (see Fig. 3). Using the notation of Fig. 3, one can write the final results in terms of real variable integrals,

$$I_n(a) = \int_{c_1}^{c_2} \frac{d\omega}{2\pi i} \left[\frac{f(i\omega + b)}{(i\omega + b)^n} - \frac{f(i\omega - b)}{(i\omega - b)^n} \right] + \int_{-b}^{b} \frac{d\omega}{2\pi i} \left[\frac{f(\omega + ic_1)}{\omega + ic_1)^n} - \frac{f(\omega + ic_2}{(\omega + ic_2)^n} \right], \tag{29}$$

where in performing the integrals along the vertical straight line we have used the substitution $z \to i\omega + b$, while for that along the horizontal path the variable becomes $z \to \omega + ic$. Now the interval (ic_1, ic_2), which contains the imaginary solution, should be searched.

6. Illustration

In what follows we shall apply the method discussed above to eliminate spurious states from RPA solutions in the case of the axially symmetric deformed superfluid nucleus ^{168}Yb. The calculations are carried out within the framework of the pairing-plus-quadrupole model (for details see Refs. [14,17]). As is clear from the previous sections, the key technical requirement for our method to be successful, is an accurate numerical integration for which we have used the routines from the NAG library.

We start analyzing the imaginary part of the response function (see Eq. (1)) with $\omega \to \omega + i\eta$), that is the quantity related to experimental observables as the scattering cross section. In Fig. 4 we show the behavior of the RPA response describing the collective modes of a deformed nucleus, that is β- and γ-vibrations. β- and γ-modes

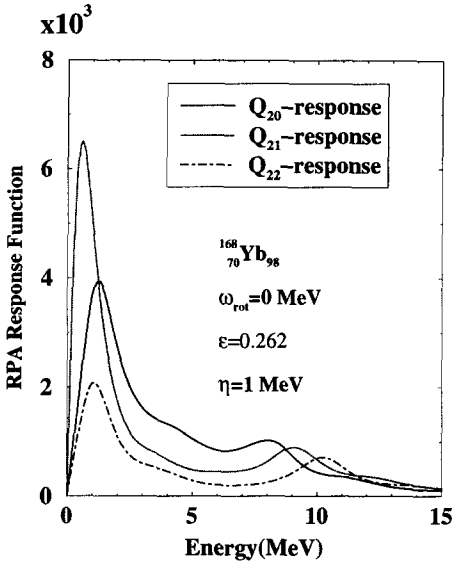

Fig. 4. $\mathrm{Im}[\mathcal{R}_{FF}(\omega + i\eta)]$ for ^{168}Yb at $\hbar\omega_{\mathrm{rot}} = 0$ MeV and for an averaging parameter $\eta = 1$ MeV. In this plot the operator $\hat{F}$ corresponds to $\hat{Q}_{20}$, $\hat{Q}_{21}$ and $\hat{Q}_{22}$. The units are defined in terms of the oscillator length $b_0^2 = \hbar/M\omega_0$ where $\hbar\omega_0 = 41.0A^{-1/3}$ MeV.

are quadrupole vibrations of the nuclear deformed shape preserving or violating axial symmetry, respectively. The projection of the angular momentum carried by the vibrations along the symmetry axis of the system associated with these modes are $K = 0$ and $K = \pm 2$. The components $K = \pm 1$ correspond to a rotation of the deformed shape around the symmetry axis, leaving the intrinsic structure of the system unchanged. For this reason the β- and γ-vibration are intrinsic states upon which rotational bands can be built.

The low-lying peak of the $\hat{Q}_{21}$ response represents the spurious contribution to the linear response function generated by the operators J_x (J_y) and related to the breakdown of rotational invariance, in keeping with the fact that $[Q_{21}, J_x]_{\mathrm{RPA}} \propto$ (deformation parameter) $\times \langle r^2 \rangle \neq 0$. However, in this energy region of the spectrum also physical solutions exist. This can be seen from Fig. 5 where the $\hat{Q}_{21}$ response is plotted for different values of the average parameters η. Already at $\eta = 0.5$ MeV (case (b) of Fig. 5) it is possible to resolve one of the low-lying physical solutions which in case (a) shows up only as a shoulder of the main peak. At the same time, the centroid of the peak associated with the spurious state moves towards $\omega = 0$ and its strength increase markedly, in keeping with the fact that the spurious state is not normalizable. The richness of the low-energy spectrum can be fully appreciated from Fig. 5(d), where a small value of the averaging parameter ($\eta = 10$ keV) has been used. The localization of the spurious states can be obtained plotting the real part of the RPA response function with $\eta = 0$ MeV because, due to its definition (see Eq. (9)), when $\omega \to \omega_n$ there is a numerical divergence in the linear response. This is shown in Fig. 6 where the

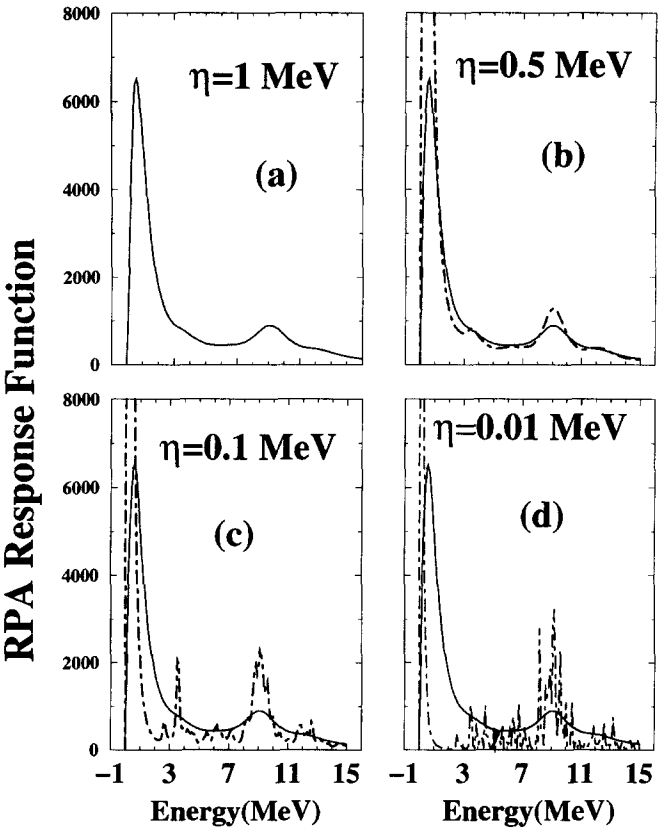

Fig. 5. $\mathrm{Im}[\mathcal{R}_{FF}(\omega + i\eta)]$ at $\hbar\omega_{\mathrm{rot}} = 0$ MeV for different values of the averaging parameter η. The operator $\hat{F}$, in all four graphs, is $\hat{Q}_{21}$. See the caption of Fig. 4 for units definition.

real part of the RPA response for the quadrupole operator $\hat{Q}_{21}$ and neutron and proton pairing operators $\hat{P}_{\tau-}$ are plotted in a small interval close to $\omega = 0$ using steps of 1 eV and $\eta = 0$ MeV. In fact, while we have already explained above the reason why the $\hat{Q}_{21}$ response represents the spurious state associated with the breakdown of rotational invariance, one has to take into account that the collective modes associated with the spontaneous breaking of gauge symmetry (particle number violation) are the pairing rotational bands. This means that the effect of the associated spurious state can be observed in the response of $\hat{P}_{\tau-} = \hat{P}_{\tau}^{\dagger} - \hat{P}_{\tau}$ operator, where $\hat{P}^{\dagger}$ is the monopole pairing operator and $\tau = n, p$ labels proton and neutron degrees of freedom, in keeping with the fact that $[\hat{N}_{\tau}, \hat{P}_{\tau-}]_{\mathrm{RPA}} = 2\Delta_{\tau} \neq 0$.

Looking at Fig. 6 one can see that, below 5 keV, there are three solutions whose intensity is divergent (cf. ordinate scale) and thus can be identified with the spurious states associated with violation of rotational invariance and proton and neutron number. Although from this calculation one cannot determine the exact energy of the spurious modes, also because such a determination will be associated with a real divergent value of the intensity, it is possible to identify quite accurately the energy interval within which

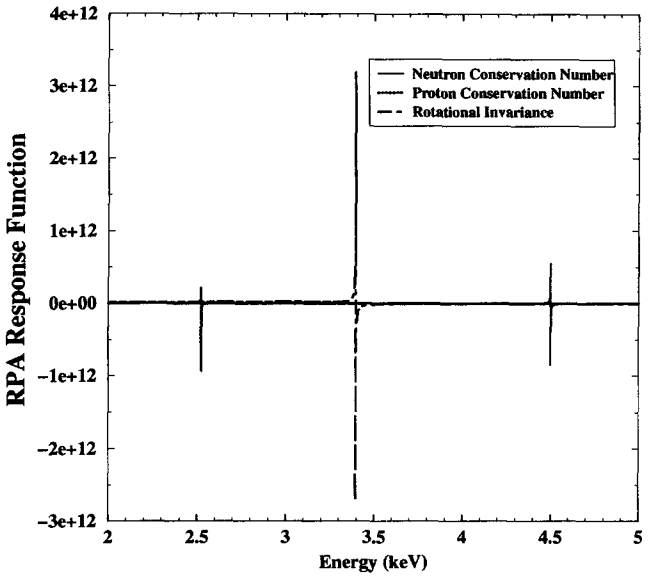

Fig. 6. Re$[\mathcal{R}_{FF}(\omega)]$ at $\hbar\omega_{\rm rot}$ = 0 MeV and η = 0. In this plot $\hat{F}$ corresponds to $\hat{Q}_{21}$, $\hat{P}_{n-}$ and $\hat{P}_{p-}$ respectively. The latter operators are dimensionless and see the caption of Fig. 4 for units definition of $\hat{Q}_{21}$.

each spurious state lies. In fact, the spurious mode associated with rotational invariance lies within the energy interval (3,4) keV while those associated with neutron- and proton-breaking of particle non-conservation lie within the intervals (2,3) keV and (4,5) keV, respectively. This information is sufficient to apply the method developed in the first part of this paper and allows the selection of appropriate values of the b-values to carry out the integration. We have a wide range of possibilities in the choice of the b-values, because the results of the integration do not depend on which specific value of b is chosen, provided it is within the correct energy interval, in keeping with the fact that the b-values define the paths of integration. After evaluating the energies and matrix elements corresponding to the spurious modes, one can subtract their contribution from the total response function and obtain the physical response function (cf. Fig. 7).

In the case of the two-neutron and two-proton transfer operators $\hat{P}_n$ and $\hat{P}_p$ one would expect that, after subtraction of the spurious states associated with the violation of particle number conservation in neutron and proton space respectively, the RPA response function still displays a consistent (physical) contribution in the energy region below 2Δ, where Δ is the value of the pairing gap, namely that associated with β-vibration. In fact, in deformed nuclei, both pairing and β-vibrations have K-quantum number equal to zero, and thus mix (cf. e.g. Ref. [18]). The fact that the remnant after subtraction of the spurious states contains a very small neutron contribution and a large proton response, is in keeping with the fact that the β-vibration in ^{168}Yb is essentially a proton mode, due to the single-particle distribution of Nilsson levels around the Fermi energy.

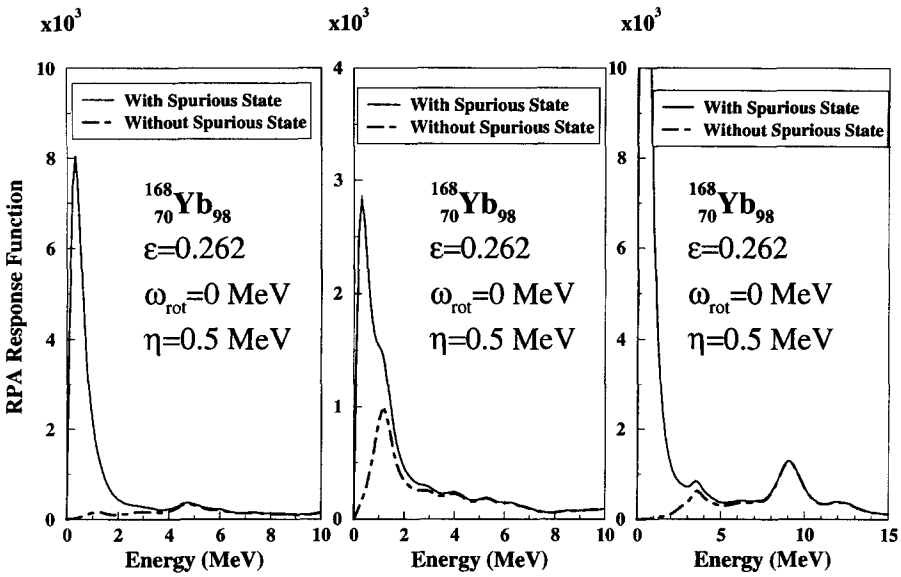

Fig. 7. Removal of the spurious modes from the $\mathrm{Im}[\mathcal{R}_{FF}(\omega+i\eta)]$ associated with broken neutron ($\hat{F} = \hat{P}_{n-}$) and proton ($\hat{F} = \hat{P}_{p-}$) gauge invariance (left and middle graphs, respectively), and rotational symmetry ($\hat{F} = \hat{Q}_{21}$) (right graph). See the caption of Fig. 6 for definition of units.

We discuss now the situation in which the spurious modes are purely imaginary, a situation we have encountered at finite rotational frequencies. A simple way to check if there exists a purely imaginary solution is to calculate the real part of the RPA response function at zero-energy with averaging parameter $\eta = 0$ MeV. Because this quantity is proportional to the IEWSR (cf. Eq. (20)), it should be a positive value, which is always fulfilled for real values of the excitation energy. Consequently, each time the real part of the linear response function at zero energy (with zero averaging parameter) has a negative value indicates that we are in presence of a complex solution of the RPA equation. The procedure to localize this imaginary solution is the same as the one for real poles (see Section 5) but this time one needs to plot the real part of RPA response using an imaginary variable $i\omega$ (as given in Fig. 8) because only in this case we have a numerical divergence in the linear response when $i\omega \to \omega_m$ (see Eq. (26)). The value of the spurious mode related to violation of neutron number conservation (Fig. 8a) lies within an energy interval centered around 1.35 keV while that associated with violation of rotational invariance lies in the interval 20 keV–30 keV (cf. Fig. 8b). The spurious mode associated with proton-number violation is, in this case, still real at finite rotational frequency. Consequently, it can be localized with the same method explained in Section 3. From Fig. 9a we see that the corresponding pole lies around 2.4 keV. Its presence can also be resolved in the rotational response Fig. 9b, even if it does not give a large contribution to the RPA response function (see different scales in graphs (a) and (b) of Fig. 9).

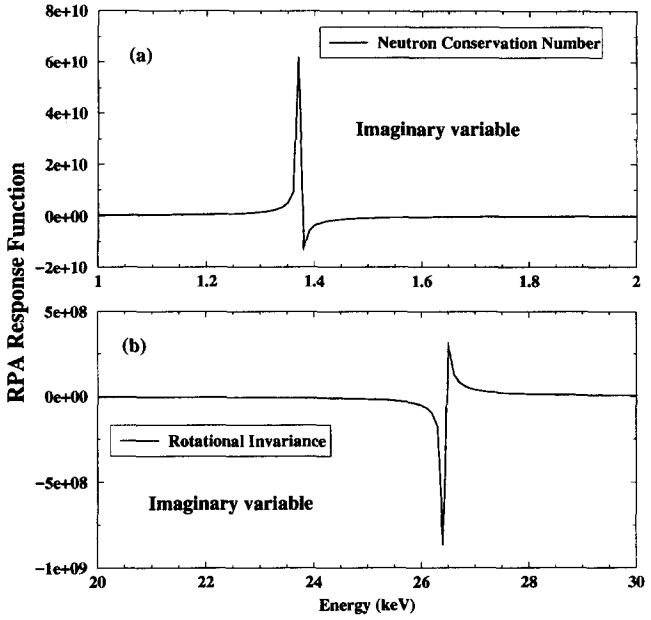

Fig. 8. Re$[\mathcal{R}_{FF}(i\omega)]$ as a function of ω when $\hat{F}$ corresponds to $\hat{P}_{n-}$ in case (a) and $\hat{Q}_{21}$ in (b) in the case of finite rotation, at $\hbar\omega_{\rm rot} = 0.4$ MeV. See the caption of Fig. 6 for units definition.

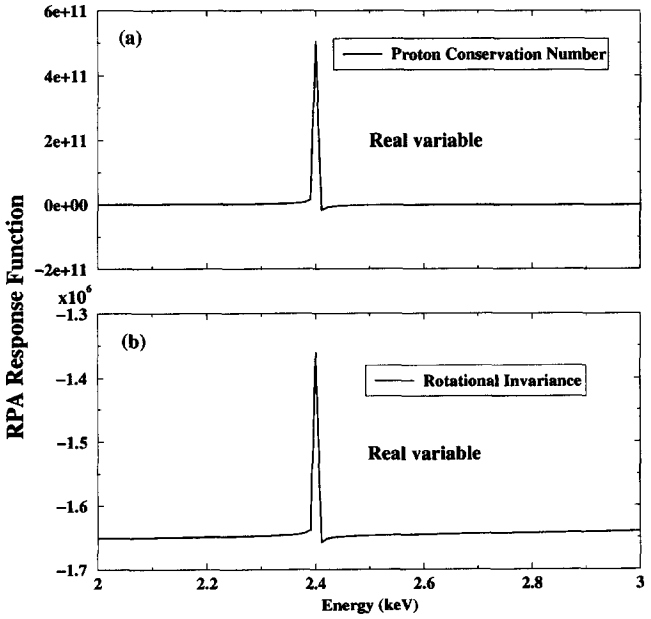

Fig. 9. Re$[\mathcal{R}_{FF}(\omega)]$ (real solutions) as a function of ω when $\hat{F}$ corresponds to $\hat{P}_{p-}$ in case (a) and $\hat{Q}_{21}$ in (b) in the case of finite rotation, $\hbar\omega_{\rm rot} = 0.4$ MeV. See the caption of Fig. 6 for units definition.

7. Conclusions

The restoration of rotational and gauge invariance symmetries spontaneously violated by mean field solutions of the nuclear Hamiltonian, implies rotations in 3D and in gauge space of the nucleus as a whole. This can be accomplished to lowest order in the coupling of the nucleonic motion to rotational motion making use of RPA. Within the framework of this "minimal" approximation the "correct" value of the associated inertias is guaranteed by the appearance of zero-frequency solutions (supernumerary, "spurious" states). The actual implementation of such a program is notoriously difficult, in particular in the case of finite rotational frequencies in 3D and gauge space. This because due to the unavoidable violation of self-consistency associated with mean field solutions, the spurious states associated with actual solutions are, although close, always shifted away from zero frequency.

A simple, yet accurate, method for carrying out the RPA program of restoration of symmetries under standard numerical situations, has been developed. It is based on linear response theory and Cauchy's integral formula, and provides energy intervals and contour paths to calculate differences of integrals of the response function which allow to evaluate and eliminate the spurious states from the spectrum of two-quasiparticle excitations, circumventing the need for a precise,a priori, knowledge of the associated poles. The method is demonstrated in the case of ^{168}Yb at finite rotational frequency.

A bonus of the technique developed in this paper is that it not only provides a compact way of eliminating the spurious states but also can be used to calculate sum rules and the whole RPA spectrum although, in the latter case, it is time consuming.

One should notice that the method was developed in the framework of a discrete RPA spectrum. When a spectrum contains a continuous part, as in the continuum RPA, the method can be applied directly because the continuum starts at excitation energy of the order of MeV and the corresponding poles deviate from the real axis (because of the natural width). In this way the spurious states are decoupled from the continuum. The removal of spurious states can become an interesting problem in situations where the continuum starts at very low excitation energy, as in the case of unstable nuclei. The extension of our technique to this situation is under study [19].

Acknowledgements

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