K

UNIVERSIDADE DE SÃO PAULO

PUBLICAÇÕES

INSTITUTO DE FÍSICA CAIXA POSTAL 20516 01498 SÃO PAULO - SP BRASIL

IFUSP/P-959

symo: 842342

REAL SOLUTION OF THE COMPLEX RANDOM PHASE APPROXIMATION EQUATION

N. Teruya and M. Kyotoku
Departamento de Física, Universidade Federal da Paraíba
C.P. 5008, 58059 João Pessoa, PB, Brasil

H. Dias Instituto de Física, Universidade de São Paulo

REAL SOLUTION OF THE COMPLEX RANDOM PHASE APPROXIMATION EQUATION

N. Teruya and M. Kyotoku

Departamento de Física, Universidade Federal da Paraíba Caixa Postal 5008 58.059 João Pessoa, PB, Brasil

H. Dias

Instituto de Física, Universidade de São Paulo Caixa Postal 20516 01498 São Paulo, SP, Brasil

ABSTRACT

The description of some nuclear collective excitations may lead to a complex eigenvalue problem of a non Hermitian matrix. It is shown that there exists a related real matrix which satisfies the usual standard real eigenvalue problem whose solution yields directly the solution of the original problem.

PACS NUMBERS: 24.30Cz, 24.30He, 21.10.Re

1. Introduction

The decay properties of giant resonances (GR's) are of special interest for the understanding of structure and dynamics of these collective modes of nuclear excitation. Since giant resonances have mostly excitation energies above particle emission thresholds they usually decay by particle emission. The total decay width consists of an "escape width", which represents the direct decay owing to the coupling of the 1p-1h doorway state to the continuum and a "spreading width" which reflects the coupling to more complicated np-nh states. The structure of GR is reasonably well understood in terms of particle-hole (p-h) configurations in the framework [1,2] of random phase approximation (RPA). The inclusion of continuum effects [3-6] in RPA calculations gives information, in principle, on direct nucleon escape.

Different discretization methods for the single particle continuum in nuclear structure calculations using RPA are currently used in the literature or are reportedly being implemented. They include projection methods in a number of variations [7-13] including the use of Weinberg "quasi-particles" [11], and the use of Gamow states [10]. Their common aim is to provide for a sound scheme allowing one to include the relevant features of the continuous single particle spectrum, notably single particle resonances with the corresponding escape widths, at reduced computational cost.

In all these discretization methods we need to solve the following, $2n \times 2n$, Complex Random Phase Approximation (CRPA) eigenvalue equation

$$\mathcal{K}\begin{pmatrix} Y \\ Z \end{pmatrix} = \omega_m \begin{pmatrix} Y \\ Z \end{pmatrix} \tag{1.1}$$

where the matrix K can take two different forms

$$\mathcal{K}_1 = \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \quad \text{or} \quad \mathcal{K}_2 = \begin{pmatrix} A & B \\ -B & -A \end{pmatrix},$$
(1.2)

A and B being complex non Hermitian matrices of order n which depend on the energy E. The eigenvector $\binom{Y}{Z}$ corresponds to the eigenvalue ω_m . The way in which these

two forms arises will not be reviewed here; our main purpose is to exhibit an equivalent real matrix for the $2n \times 2n$ CRPA eigenvalue equation. It is important to mention that our method does not make any difference if the size of the matrix is small but, if our shell basis includes two major shells in the lead region, it is worthwhile to apply the technique developed in the present paper, where in section 2 the formalism is presented with some applications given in section 3. Some conclusions are drawn in section 4.

2. Transformation of CRPA equation to the real eigenvalue problem

As we mentioned before, eq. (1.1) is simply an eigenvalue equation of the type $\mathcal{KX} = \omega_m \mathcal{X}$ with $\mathcal{K} \in \mathbf{C}_{2n}$ where \mathbf{C}_{2n} means a complex square matrix of 2n rows. Here it is worthwhile to mention that the usual library subroutines diagonalize an equivalent $4n \times 4n$ real matrix. This eigenvalue equation can be solved with the help of the already existing subroutines, that one can find, for example, in the NAG or IMSL subroutines libraries [14].

However, noticing the block structure of the CRPA matrices, it is interesting to see whether K can be transformed in such way that we find an equivalent real matrix. To reach this goal let us multiply both sides of eq. (1.1) by K, then after some trivial manipulation we obtain

$$\begin{pmatrix} A & -B \\ -B^* & A^* \end{pmatrix} \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} Y \\ Z \end{pmatrix} = \omega_m^2 \begin{pmatrix} Y \\ Z \end{pmatrix}. \tag{2.1}$$

Applying now the following unitary transformation

$$J = \frac{1}{\sqrt{2}} \begin{pmatrix} I & I \\ -iI & iI \end{pmatrix} , \qquad (2.2)$$

where I is the identity matrix; for to the eigenvalue problem (2.1) we get

$$\begin{pmatrix} \operatorname{Re} \mathcal{D}^{-} & -\operatorname{Im} \mathcal{D}^{+} \\ \operatorname{Im} \mathcal{D}^{-} & \operatorname{Re} \mathcal{D}^{+} \end{pmatrix} \begin{pmatrix} \operatorname{Re} \mathcal{D}^{+} & -\operatorname{Im} \mathcal{D}^{-} \\ \operatorname{Im} \mathcal{D}^{+} & \operatorname{Re} \mathcal{D}^{-} \end{pmatrix} \begin{pmatrix} m \\ n \end{pmatrix} = \omega_{m}^{2} \begin{pmatrix} m \\ n \end{pmatrix}. \tag{2.3}$$

where Re(Im) \mathcal{D}^{\pm} = Re(Im) [A \pm B] (2.4)

and

3

$$\binom{m}{n} = J\binom{Y}{Z} \ . \tag{2.4}$$

It is interesting to note here that, if Im $\mathcal{D}^{\pm}=0$, we get back to the $\mathrm{Chi}^{[15]}$ formalism for solving the real RPA equation. He originally transformed the 2n real RPA eigenvalue equation to the n symmetric eigenvalue equation, which can be solved by well-known and reliable methods. In the present case, the 2n complex eigenvalue equation can be further transformed to the 2n real eigenvalue equation. However, we can use this method to transform the second eigenvalue equation presented in eq. (1.2). Therefore, if we apply the following orthogonal transformation

$$J' = \frac{1}{\sqrt{2}} \begin{pmatrix} I & I \\ -I & I \end{pmatrix} , \qquad (2.5)$$

to the matrix \mathcal{K}_2 , we get

$$J^{\prime\dagger}\mathcal{K}_{2}J^{\prime} = \begin{pmatrix} 0 & A+B \\ A-B & 0 \end{pmatrix} \equiv \mathcal{K}_{2}^{\prime} . \tag{2.6}$$

The eigenvalue equation (1.1) takes the following new form

$$\mathcal{K}_2'\binom{\alpha}{\beta} = \omega_m \, \binom{\alpha}{\beta},\tag{2.7}$$

where

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = J'^{\dagger} \begin{pmatrix} Y \\ Z \end{pmatrix} . \tag{2.8}$$

Multiplying again the above eigenvalue equation (2.7) by \mathcal{K}_2' we get two uncoupled eigenvalue equations of the type

$$C\alpha \equiv (A+B)(A-B)\alpha = \omega_m^2 \alpha \tag{2.9a}$$

$$D\beta \equiv (A-B)(A+B)\beta = \omega_m^2 \beta \tag{2.9b}$$

It is worthwhile to mention that the above two equations were obtained by $Chi^{[15]}$ for the case where A and B were both real. As one can also note, the previous problem of the

diagonalization of the complex matrix of the order 2n is transformed into the problem of an n order complex matrix, which obviously means that we simplify our original problem. However, we can simplify further by defining the following 2n complex matrix eigenvalue equation extended from (2.9a) which is similar to the \mathcal{K}_1 from Eq. (1.2)

$$P\begin{pmatrix} p \\ p_c \end{pmatrix} \equiv \begin{pmatrix} C & 0 \\ 0 & C^* \end{pmatrix} \begin{pmatrix} p \\ p_c \end{pmatrix} = \xi \begin{pmatrix} p \\ p_c \end{pmatrix} \tag{2.10}$$

Using now the unitary transformation (2.4)

$$P_{J} \equiv JPJ^{\dagger} = \begin{pmatrix} \operatorname{Re} C & -\operatorname{Im} C \\ \operatorname{Im} C & \operatorname{Re} C \end{pmatrix}$$
 (2.11)

which is a real matrix of 2n order. The eigenfunctions from (2.9) are also transformed into

$$\gamma_j \equiv J \begin{pmatrix} p \\ p_c \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} p + p_c \\ -i(p - p_c) \end{pmatrix} \tag{2.12}$$

Therefore, the original complex eigenvalue equation is now equivalent to

$$P_J \gamma_i = \xi \gamma_j. \tag{2.13}$$

By comparison of eq.(2.13) with eq.(2.9), we have $\xi = \omega_m^2$ with $p_c = 0$ and $\xi = \omega_m^{*2}$ with p = 0. For the first solution we have from (2.7)

$$\beta = \frac{1}{\omega_m} (A - B)\alpha; \tag{2.14}$$

replacing this expression in eq.(2.8) and with the help of (2.2) we get the following form for the original eigenvector

$$\begin{pmatrix} Y \\ Z \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} I + \omega_m^{-1}(A - B) \\ -I + \omega_m^{-1}(A - B) \end{pmatrix} \begin{pmatrix} p \\ p \end{pmatrix}$$
 (2.15)

Therefore, as before, the original problem of diagonalizing a 2n complex matrix is simplified by the diagonalization of a 2n real matrix which has more reliable subroutines available.

3. Numerical Tests

Let us present now two numerical tests in order to verify our formalism by introducing the following matrices A and B from the CRPA equation (1.1)

$$A = \begin{pmatrix} 16.367 & -0.900i & -4.277 & 0.000i \\ -4.277 & 0.000i & 9.967 & -0.200i \end{pmatrix}$$

and

$$B = \begin{pmatrix} .670 & 0.000i & 3.055 & 0.000i \\ 3.055 & 0.000i & .670 & 0.000i \end{pmatrix}$$

As one can see in the above matrices, the complex numbers are only in the diagonal elements of the matrix A; however, we have also verified our method for any complex matrices A and B. Then, using the above matrices to perform the matrix product (2.3) we can find a real matrix which is diagonalized through a standard subroutine from IMSL called EIGRF, furnishing the following eigenvalues,

$$\omega_1 = 18.28834 - 0.75708i$$
 and $\omega_2 = 7.04366 - 0.34292i$.

The eigenvectors obtained from the inverse transformation of (2.4) for the eigenvalues ω_1 and ω_2 , are, respectively,

$$\begin{pmatrix} Y_1^1 \\ Y_2^1 \\ Z_3^1 \\ Z_4^1 \end{pmatrix} = \begin{pmatrix} 0.89273 - 0.01216i \\ -0.45924 - 0.02359i \\ 0.01290 + 0.00233i \\ -0.08367 + 0.00058i \end{pmatrix}$$

and

$$\begin{pmatrix} Y_1^2 \\ Y_2^2 \\ Z_3^2 \\ Z_4^2 \end{pmatrix} = \begin{pmatrix} 0.47963 + 0.02393i \\ 0.90731 - 0.01263i \\ -0.16170 + 0.00405i \\ -0.16249 - 0.00415i \end{pmatrix}$$

The above values can be compared to those obtained through direct diagonalization of the complex matrix with a IMSL subroutine called EIGCC, furnishing

$$\omega_1 = 18.28822 - 0.75708i \text{ with } \begin{pmatrix} Y_1^1 \\ Y_2^1 \\ Z_3^1 \\ Z_4^1 \end{pmatrix} = \begin{pmatrix} 0.89273 - 0.01216i \\ -0.45924 - 0.02359i \\ 0.01290 + 0.00233i \\ -0.08367 + 0.00058i \end{pmatrix}$$

and

$$\omega_2 = 7.04357 - 0.34292i \quad \text{with} \quad \begin{pmatrix} Y_1^2 \\ Y_2^2 \\ Z_3^2 \\ Z_4^2 \end{pmatrix} = \begin{pmatrix} 0.47963 + 0.02393i \\ 0.90731 - 0.01263i \\ -0.16170 + 0.00405i \\ -0.16249 - 0.00415i \end{pmatrix}.$$

As expected, there is a neglible difference between the two results in the real part of the eigenvalues. The imaginary part of the eigenvalues and the eigenvectors are almost the same. The second, and final, verification of the CRPA equation (1.1) with \mathcal{K}_2 is now presented. We diagonalized the equivalent real eigenvalue equation (2.11) and we found

$$\omega_1 = 18.28846 - 0.76017i$$
 and $\omega_2 = 7.04672 - 0.40037i$.

Now, the eigenvectors are obtained from (2.15) for the eigenvalues ω_1 and ω_2 , resulting, respectively,

$$\begin{pmatrix} Y_1^1 \\ Y_2^1 \\ Z_3^1 \\ Z_t^1 \end{pmatrix} = \begin{pmatrix} 0.89272 - 0.01210i \\ -0.45926 - 0.02369i \\ 0.01275 + 0.00287i \\ -0.08366 - 0.00054i \end{pmatrix}$$

and

$$\begin{pmatrix} Y_1^2 \\ Y_2^2 \\ Z_3^2 \\ Z_4^2 \end{pmatrix} = \begin{pmatrix} 0.47943 + 0.02621i \\ 0.90706 - 0.00967i \\ -0.16102 - 0.01076i \\ -0.16183 - 0.01274i \end{pmatrix}$$

As before, these values can be compared to those obtained through direct diagonalization of the complex matrix with the above mentioned subroutine

$$\omega_1 = 18.28835 - 0.76016i \text{ with } \begin{pmatrix} Y_1^1 \\ Y_2^1 \\ Z_3^1 \\ Z_4^1 \end{pmatrix} = \begin{pmatrix} 0.89272 - 0.01210i \\ -0.45926 - 0.02369i \\ 0.01275 + 0.00287i \\ -0.08366 - 0.00054i \end{pmatrix}$$

and

$$\omega_2 = 7.04665 - 0.40036i \text{ with } \begin{pmatrix} Y_1^2 \\ Y_2^2 \\ Z_3^2 \\ Z_4^2 \end{pmatrix} = \begin{pmatrix} 0.47944 + 0.02621i \\ 0.90706 - 0.00967i \\ -0.16102 - 0.01076i \\ -0.16183 - 0.01274i \end{pmatrix}$$

Here, as we previously mentioned, there is still a small difference between the two results in the real and imaginary part of the eigenvalues, which was the same in the latter diagonalization. Here the eigenvectors are almost the same. Finally, we would like to comment that we present only one of the eigenvalues and eigenvectors, which are normalized. It is also worthwhile to mention that all the calculations presented were performed in a IBM 4381 with 16MB.

4. Conclusion

The CRPA eigenvalue eigenfunctions which appear, respectively, before or after projecting the continuum spectrum is solved by transforming to an equivalent real eigenvalue equation. This operation reduces the size of the matrix to be diagonalized and increases the reliability of the final results.

Acknowledgments

We would like to thank W.A. Seale for a critical reading of the manuscript. This work was supported in part by the Conselho de Desenvolvimento Científico e Tecnológico (CNPq).

5. References

- [1] G.E. Brown, Unified Theory of Nuclear Models (North Holland, Amsterdam, 1964).
- [2] A. Bohr and B.R. Mottelson, Nuclear Structure, Vol. II (Benjamin, Reading, 1975).
- [3] G.F. Bertsch and S.F. Tsai, Phys. Rep. 18C (1975) 125.
- [4] K.F. Liu and G.E. Brown, Nucl. Phys. A265 (1976) 385.
- [5] S. Krewald, V. Klempt, J. Speth and A. Faessler, Nucl. Phys. A281 (1977) 166.
- [6] G.A. Rinker and J. Speth, Nucl. Phys. A306 (1978) 360.
- [7] W.L. Wang and C.M. Shakin, Phys. Lett. 32B (1970) 421.
- [8] S. Yoshida and S. Adachi, Nucl. Phys. A457 (1986) 84.
- [9] F. Zardi and P.F. Bortignon, Europhys. Lett. 1 (1986) 281; N.V. Giai, P.F. Bortignon, F. Zardi and R.A. Broglia, Phys. Lett. 199B (1987) 155.
- [10] T. Vertse, P. Curutchet, O. Civitarese, L.S. Ferreira and R.J. Liotta, Phys. Rev. C37(1988) 876; P. Curutchet, T. Vertse and R.J. Liotta, Phys. Rev. C39 (1987) 1020.
- [11] M. Buballa, A. Gattone, R. de Haro, R. Jessenberger and S. Krewald, Nucl. Phys. A517 (1990) 61; See S. Weinberg, Phys. Rev. 133 (1964) 232.
- [12] S. Drodzd, G. Co, J. Wambach and J. Speth, Phys. Lett. 199B (1987) 155.
- [13] A.F.R. de Toledo Piza, Rev. Bras. Fis. 17 (1987) 195; N. Teruya, A.F.R. de Toledo Piza and H. Dias, Phys. Rev. C44 (1991) 537; N. Teruya, H. Dias and A.F.R. de Toledo Piza, Proc. of the International Nuclear Physics Conference, 1989, São Paulo, page p5-52.
- [14] Fortran Routines Mark10 Numerical Algorithm Group (NAG), Oxford UK and Illinois USA; User's Manual, IMSL Math/Library, USA.
- [15] B. Chi, Nucl. Phys. A146 (1970) 449.