Core polarization effects and the random phase approximation solution

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Abstract. Simplified formulae for the effective electromagnetic transition matrix elements and the core polarization contribution to the effective two-nucleon interaction are derived. From these general expressions, the polarization effects in any other physical quantity of interest can easily be written down. It is also proved that the usual RPA eigenvalue problem corresponding to a $2n \times 2n$ matrix $\begin{pmatrix} A & B \\ -B & -A \end{pmatrix}$ is equivalent to the diagonalization of a $n \times n$ matrix $(A + B)\,(A - B)$.

Keywords. Core nucleus; valence nucleons; random phase approximation; core polarization effects.

1. Introduction

Shell model calculations are carried out with the consideration of a few active nucleons confined to a finite model space. The rest of the nucleons in the nucleus form a passive core. The effect of both the assumptions of the passive core and of the finite model space is incorporated by introducing effective charges to explain electromagnetic transitions and moments, and by renormalizing the two-nucleon interaction to explain the low-lying spectra of nuclei. The contribution to a given matrix element arising from the virtual excitations of the core state is usually referred to as the 'core polarization' contribution. Existence of collective modes of oscillations of the core nucleus plays an important role in understanding these polarization effects. Recently, the concept of effective operators has received much attention through the point of view of understanding the spectroscopic results of lighter nuclei in the doubly-magic region (Rowe 1973, Satchler 1972, Ellis and Osnes 1972, Osnes *et al* 1971).

The microscopic approach to the shell model calculations for the open shell nuclei starts with the Brueckner-Bethe theory. The effective interaction between two nucleons in a nucleus is taken to be the G matrix (appropriate for the core nucleus) derived from realistic nucleon-nucleon force, such as the Hamada-Johnston force. Using this G, the core-polarization contribution to any matrix element corresponding to a given physical process of interest is calculated in the random phase approximation (RPA), Tamm-Dancoff approximation (TDA) and with the unperturbed description of the core nucleus.

2. Formalism

The study of core polarization effects is based on the many-body perturbation theory, the unperturbed Hamiltonian being the sum of the core nucleons Hamiltonian and the valence nucleons one. The configuration space over which these Hamiltonians are defined has no common intersection. The core states are obtained by solving the RPA eigenvalue problem. The valence nucleon wave functions are the eigenfunctions of the one-body shell model Hamiltonian. The RPA eigenvalues and the eigenvectors are obtained by solving the matrix equation

$$\begin{pmatrix} A(\lambda t) & B(\lambda t) \\ -B(\lambda t) & -A(\lambda t) \end{pmatrix} \begin{pmatrix} X_n \\ Y_n \end{pmatrix} = h(\lambda t) \begin{pmatrix} X_n \\ Y_n \end{pmatrix} = \omega_n(\lambda t) \begin{pmatrix} X_n \\ Y_n \end{pmatrix} \tag{1}$$

The matrices $A(\lambda t)$ and $B(\lambda t)$ are defined as follows

$$\langle ph \mid A(\lambda t) \mid p'h' \rangle = (\epsilon_p - \epsilon_h)\, \delta_{pp'}\, \delta_{hh'} + (-1)^{p'-h'+\lambda+t}\, G(h'p'\,[\lambda t];\; ph)$$

and

$$\langle ph \mid B(\lambda t) \mid p'h' \rangle = (-1)^{p'-h'+\lambda+t}\, G(p'h'\,[\lambda t];\; ph) \tag{2}$$

The particle-hole coupled matrix elements in eq. (2) are defined in terms of the effective interaction G, calculated from the Brueckner-Bethe-Goldstone theory for the core nucleus,

$$G(fi\,[\lambda t];\; ph) = (-1)^{p-h+\lambda+t}\, [(1+\delta_{fp})(1+\delta_{ih})]^{\frac{1}{2}} \times \sum_{JT} (2J+1)(2T+1) \begin{bmatrix} f & i & \lambda \\ h & p & J \end{bmatrix} \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & t \\ \frac{1}{2} & \frac{1}{2} & T \end{bmatrix} \langle fpJT \mid G \mid ihJT \rangle \tag{3}$$

The notation p, h, f and i is used in the phase factor and in the six-j symbol stand for corresponding total angular momentum values j_p, etc.; elsewhere, they indicate all the quantum numbers necessary for the specification of shell mode states.

Polarization effects are calculated from the second order perturbation theory in the coupling of the valence nucleons. Its contribution to the electromagnetic transition caused by an operator $O(\lambda t)$ comes from the two diagrams shown in figure 1. The multi-polarity and the isospin character of the operator O are indicated

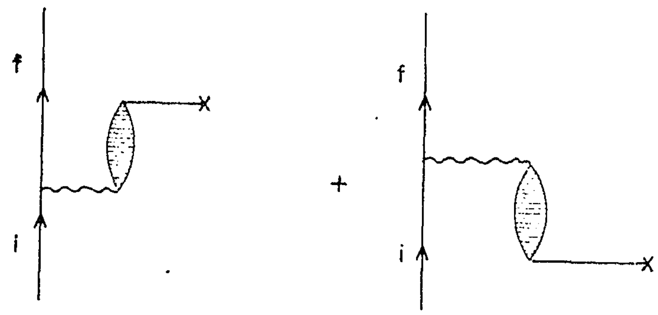

Figure 1. Core polarization contribution to the electromagnetic transition. The wavy lines represent antisymmetrized G-matrix elements and the cross-hatched bubbles the RPA description of the core. Straight line with a cross at the end indicates the external electromagnetic interaction caused due to the operator $O(\lambda t)$

by λ and t respectively. The effective transition matrix element is defined as the sum of the transition matrix element of the electromagnetic interaction with the valence nucleons and the core polarization contribution.

Following the method of Osnes and Warke (1969) the total core polarization contribution to the transition amplitude can easily be written down from figure 1 (Ellis and Osnes 1972).

$$(f\| O_{pol}(\lambda t) \| i)$$
$$= (-1)^{\lambda+t} \sum_n [\epsilon_{if} - \omega_n(\lambda t)]^{-1} x_{n,\lambda t}(fi)$$
$$\times \sum_{ph} (-1)^{p-h} [X_{n,\lambda t}(ph) + Y_{n,\lambda t}(ph)] \langle h \| O(\lambda t) \| p \rangle$$
$$+ \{i \leftrightarrow f\} (-1)^{f-i} \tag{4}$$

where

$$x_{n,\lambda t}(fi) = \sum_{ph} [X_{n,\lambda t}(ph)\, G(fi[\lambda t];\ ph) + Y_{n,\lambda t}(ph)\, G'(fi[\lambda t];\ ph)].$$

In equation (4), $\epsilon_{if} = \epsilon_i - \epsilon_f$, denotes the energy difference of valence nucleons and the reduced matrix element is defined both with respect to angular momentum and isospin reduction. The vector $G'(fi[\lambda t])$ is defined in terms of the particle-hole coupled matrix elements in eq. (3)

$$G'(fi[\lambda t];\ ph) = (-1)^{f-i}\, G(if[\lambda t];\ ph) \tag{5}$$

Defining the vector $\mathbf{O}(\lambda t,\ ph) = (-1)^{p-h} \langle h \| \mathbf{O}(\lambda t) \| p \rangle$, it can be seen that eq. (4) takes the following vector product form,

$$(f \| O_{pol}(\lambda t) \| i)$$
$$= (-1)^{\lambda+t} (\tilde{O}(\lambda t)\ \tilde{O}(\lambda t)) \frac{1}{\epsilon_{if} - h(\lambda t)} \times \begin{pmatrix} G(fi[\lambda t]) \\ -G'(fi[\lambda t]) \end{pmatrix} \tag{6}$$

In the derivation of eq. (6) use is made of the completeness of RPA eigenvectors. Further, if one evaluates the inverse of the matrix $\epsilon_{if} - h[\lambda t]$ in eq. (6) and carries out the matrix products, it reduces to

$$(f \| O_{pol}(\lambda t) \| i)$$
$$= (-1)^{\lambda+t} \{\tilde{O}(\lambda t)\, M_{if}^{-1}(\lambda t)\, [A(\lambda t) - B(\lambda t)]$$
$$\times [G(fi[\lambda t]) + G'(fi[\lambda t])] - \epsilon_{if}\tilde{O}(\lambda t)\, M_{if}^{-1}(\lambda t)$$
$$\times [G(fi[\lambda t]) - G'(fi[\lambda t])]\} \tag{7}$$

where the matrix

$$M_{if}(\lambda t) = [A(\lambda t) - B(\lambda t)]\, [A(\lambda t) + B(\lambda t)] - \epsilon_{if}^2 \tag{8}$$

For the case of $\epsilon_{if} = 0$, the core polarization contribution in eq. (7) becomes;

$$(-1)^{\lambda+t}\, \tilde{O}(\lambda t)\, [A(\lambda t) + B(\lambda t)]^{-1} [G(fi[\lambda t]) + G'(fi[\lambda t])] \tag{9}$$

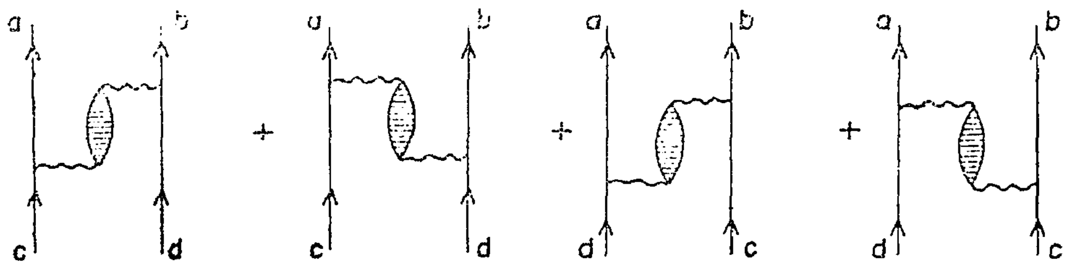

Figure 2. Core polarization of a fully antisymmetric two-particle matrix element. The wavy line represents G-matrix elements and the cross-hatched bubbles the RPA description of the core.

After performing a little bit of matrix algebra, the above result can also be obtained from the Barrett and Kirson (1970) formula. Following a similar approach, the core polarization contribution to the effective interaction given by Osnes and Warke cannot be simplified. However, the formulae derived by Kirson (1971) can be put in a much simpler form. This difference between the two methods is due to the fact that when $\epsilon_{if} \neq 0$, the polarization contribution to the effective interaction does not satisfy

$$(ab \mid G_{\text{phonon}}(JT) \mid cd) = (cd \mid G_{\text{phonon}}(JT) \mid ab) \tag{10}$$

while this equality is true for $\epsilon_{if} = 0$. In what follows, we define the core polarization contribution as

$$\begin{aligned}(ab \mid G_{\text{pol}}(JT) \mid cd)\\ = \tfrac{1}{2}\left[(ab \mid G_{\text{phonon}}(JT) \mid cd) + (cd \mid G_{\text{phonon}}(JT) \mid ab)\right]\end{aligned} \tag{11}$$

As discussed by Osnes, Kuo and Warke (1971), the contribution to each matrix element of G_{phonon} comes from four diagrams shown in figure 2. Thus there would be eight terms in eq. (11). Out of these, we consider the sum of only two terms; rest of the contribution can easily be written down from our final result. The contribution of the first diagram coming from each term of eq. (11) is

$$\begin{aligned}(ab \mid G_{\text{pol}}(J'T') \mid cd)_1 = \tfrac{1}{2}\left[(1+\delta_{ab})(1+\delta_{cd})\right]^{-\frac{1}{2}}(-1)^{J'+T'+1} \times\\ \times \sum_{n,J,T} \begin{bmatrix} a & b & J' \\ d & c & J \end{bmatrix} \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & T' \\ \frac{1}{2} & \frac{1}{2} & T \end{bmatrix} \left[\left\{\frac{(-1)^{b+c}\, x_{n,JT}(ac)\, x'_{n,JT}(bd)}{\epsilon_{ca} - \omega_n(JT)}\right\} + \{a, b \leftrightarrow c, d\}\right]\end{aligned} \tag{12}$$

Here $x'_{n,JT}(bd)$ is defined with the interchange of G' and G in eq. (4), defining $x_{n,JT}(bd)$. Using again the completeness relation of the RPA eigenvectors and the following relation between the vectors G' and G

$$G'(ac\,[JT]; ph) = (-1)^{c-a}\, G(ca\,[JT]; ph) \tag{13}$$

it can be shown that the two terms in the square bracket of eq. (12) become

$$(-1)^{b+c}\left(G'(bd\,[JT])\, \tilde{G}(bd\,[JT])\right) \frac{1}{\epsilon_{ca} - h(JT)} \begin{pmatrix} G(ac\,[JT]) \\ -G'(ac\,[JT]) \end{pmatrix} \tag{14}$$

With the substitution of the inverse of the matrix, $\epsilon_{ca} - h(JT)$ the matrix product (14) reduces to

$$(-1)^{b+c}\Big[\{\tilde{G}(bd\,[J\,T]) + \tilde{G}'(bd\,[J\,T])\}\, M_{ca}^{-1}(J\,T)\,(A\,(J\,T) - B\,(J\,T))$$
$$\times \{G\,(ac\,[J\,T]) + G'\,(ac\,[J\,T])\}$$
$$- \{\tilde{G}\,(bd\,[JT]) - \tilde{G}'\,(bd\,[JT])\}\, \tilde{M}_{ca}^{-1}(J\,T)\,(A\,(J\,T) + B\,(J\,T))$$
$$\times \{G\,(ac\,[JT]) - G'\,(ac\,[JT])\}$$
$$- \epsilon_{ca}\{\tilde{G}\,(bd\,[JT]) + \tilde{G}'\,(bd\,[JT])\}\, M_{ca}^{-1}(JT)\,\{G\,(ac\,[JT])$$
$$- G'\,(ac\,[J\,T])\} + \epsilon_{ca}\{\tilde{G}\,(bd\,[J\,T]) - \tilde{G}'\,(bd\,[J\,T])\}$$
$$\times \tilde{M}_{ca}^{-1}(J\;T)\{G\,(ac\,[J\,T]) + G'\,(ac\,[J\,T])\}\Big] \tag{15}$$

Using the expression in eq. (15) for the square bracket in eq. (12), we obtain the final form of the polarization contribution to the effective nucleon-nucleon interaction in a nucleus. The rest of the contribution coming from the other three diagrams can be written down from eqs (12) and (15) by simply interchanging indices $a \leftrightarrow b$ and $c \leftrightarrow d$. In the case of $\epsilon_{ca} = 0$, the polarization contribution in eq. (12) takes a very simple form,

$$(ab|G_{pol}\,(J'\,T')\,|\,cd)_1$$
$$= \tfrac{1}{2}\,[(1+\delta_{ab})\,(1+\delta_{cd})]^{-1/2}\,(-1)^{J'+T'+b-c}$$
$$\times \sum_{JT} \begin{bmatrix} a\; b\; J' \\ d\; c\; J \end{bmatrix} \begin{bmatrix} \frac{1}{2}\; \frac{1}{2}\; T' \\ \frac{1}{2}\; \frac{1}{2}\; T \end{bmatrix} \{[\tilde{G}\,(bd\,[J\,T]) + \tilde{G}'\,(bd\,[JT])]$$
$$\times [A\,(JT) + B\,(JT)]^{-1}\,[(G\,(ac\,[J\,T]) + G'\,(ac\,[JT])]$$
$$- [(\tilde{G}\,(bd\,[JT]) - \tilde{G}'\,(bd\,[JT])]\,[A\,(J\,T) - B\,(JT)]^{-1}$$
$$\times [(G\,(ac\,[JT]) - G'\,(ac\,[JT])]\} \tag{16}$$

We have seen that Barrett and Kirson's (1970) expression for the polarization contribution to the effective interaction also takes this form. From eqs (12) and (15), one can write down the core polarization contribution to any matrix element for a physical process of interest by simply replacing the corresponding G and G' on both the left and the right hand sides of eq. (15).

The form of the matrix M in eqs (7) and (15) suggests that the RPA equations may be equivalent to the eigenvalue problem corresponding to the matrices $(A+B)(A-B)$ and $(A-B)(A+B)$. In fact with simple algebra, one can prove that

$$\left[Det\begin{pmatrix} A-\omega & B \\ -B & -A-\omega \end{pmatrix}\right]^2$$
$$= Det\,[(A+B)\,(A-B) - \omega^2]$$
$$\times\, Det\,[(A-B)\,(A+B) - \omega^2)] \tag{17}$$

In deriving eq. (17), we used the result that the RPA eigenvalues occur in pairs $\pm\,\omega_n$. This implies that the determinant on the right hand side of eq. (17) is an even function of ω. The two determinants on the right hand side of this equation are equal since the corresponding matrices are the transpose of each other. Thus, we proved that the eigenvalues of the $2n \times 2n$ RPA matrix are given by the square roots of the eigenvalues of the matrix $(A + B)(A - B)$ [or of the matrix $(A - B) \times (A + B)$]. From this result one also infers that this matrix may be related to the square of the RPA matrix. In fact, this eigenvalue problem is exactly identical with the diagonalization of $(A + B)(A - B)$ and $(A - B)(A + B)$. Let us denote the eigenvectors of the matrix $(A + B)(A - B)$, corresponding to the eigenvalues ω_n^2 by u_n. Since this matrix is not hermitian, u_n's do not satisfy the usual orthonormality relations. It is easy to show that $v_n = (A - B)\, u_n / \omega_n$ are the eigenvectors of the matrix $(A - B)\ (A + B)$ with the eigenvalue ω_n^2. Using the eigenvalue equations of u_n and v_n, one obtains the orthonormality relations

$$\tilde{v}_n\, u_m = \delta_{nm} \tag{18}$$

The RPA eigenvectors corresponding to the eigenvalues ω_n are then given by

$$\left.\begin{aligned} X_n &= \tfrac{1}{2}\,[u_n + (A - B)\, u_n/\omega_n] \\ &\text{and} \\ Y_n &= \tfrac{1}{2}\,[u_n - (A - B)\, u_n/\omega_n] \end{aligned}\right\} \tag{19}$$

The relation in eq. (18) ensures the usual orthonormality relations of the RPA vectors. This method of solving the $2n \times 2n$ RPA matrix eigenvalue problem requires the solution of only one $n \times n$ matrix diagonalization. This would make it possible to extend the study of the collective states of nuclei in the heavier mass region with the inclusion of reasonably large particle-hole space. A rather different approach for the RPA eigenvalue problem was also suggested by Chi (1970).

The derivation of eqs (7) and (15) depends on the assumption of a non-zero eigenvalue of the RPA equations (particularly the case of $\epsilon_{ij} = 0$). It would be interesting to generalize the above approach for this case.

3. Results and conclusion

The merit of our formulae is that the core polarization contributions are calculated from only the knowledge of a $n \times n$ inverse matrix, M^{-1}. The laborious job of calculating and storing the RPA eigenvalues and the eigenvectors is avoided. Even though this was not the difficulty in Barrett and Kirson's method, one still had to evaluate inverse of the matrices which were really not needed. Besides this, they have to take $\epsilon_{ij} = 0$, in which case our expression (16) is extremely simple. Because of the numerical difficulties involved, such calculations are carried out only for ^{16}O and ^{40}Ca nuclei, that too with a moderate particle-hole space to construct A and B matrices. This approach would allow us to extend such studies in the nuclei of heavier mass region. One can even include the larger particle-hole space. In the TDA and the unperturbed description of the core, this contribution can be obtained simply by setting $B(JT) = 0$, and $B(JT) = 0$ and $A(JT) = (\epsilon_p - \epsilon_n)$ respectively. Inclusion of particle-hole vertex and propagator corrrection can be introduced by simply redefining the matrices $A(JT)$ and $B(JT)$ in eq. (15). The effect of the renormalization of the outer vertex considered by Kirson (1971) changes only the matrices G and G' in eq. (15).

The reduction of the RPA eigenvalue problem to a $n \times n$ matrix diagonalization would make it possible to extend the study of the collective states of nuclei in the heavier mass region.

References

Barrett B R and Kirson M W 1970 *Nucl. Phys. A* **145** 145.

Chi B 1970 *Nucl. Phys. A* **146** 449

Ellis P J and Osnes E 1972 *Phys. Lett. B* **42** 335

Ellis P J and Osnes E 1972 *Phys. Lett. B* **41** 97

Kirson M W 1971 *Ann. Phys.* **66** 624

Osnes E, Kuo T T S and Warke C S 1971 *Phys. Lett. B* **34** 113

Osnes E, Kuo T T S and Warke C S 1971 *Nucl. Phys. A* **168** 190

Osnes E and Warke C S 1969 *Phys. Lett. B* **30** 306

Rowe D J 1973 *Phys. Lett. B* **44** 155

Satchler G R 1972 *Comments Nucl. Particle Phys.* **5** 145