THE SPURIOUS STATES PROBLEM AND AN EXTENSION OF THE RPA (*)

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ABSTRACT — Corrections to RPA transition amplitudes arising from ground state correlations due to the zero point motion of the several degrees of freedom have been considered elsewhere. Since a complet set of states was required in the derivations the zero point motion of the spurious degrees of freedom was also involved in the expressions obtained for transition amplitudes. It is shown here that the contribution of the spurious states actually cancels out in those expressions if the transition operator commutes with colective operators such as center of mass position and total momentum.

1 — INTRODUCTION

Corrections to RPA transition amplitudes arising from ground state correlations have been considered in other papers (1, 2, 3). Those corrections involve spurious states. Corrections to one-phonon transition amplitudes, for instance, contain summations extending over all RPA bosons, which may be regarded as arising from the zero-point motion of the several degree of freedom. Since a complete set of states was required in the derivations, the so called spurious states had to be included in the summations. However, the exact center of

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mass and orientation wave packets are obviously unimportant for intrinsic excitations, so one expects the contribution of the spurious states to cancel out. In section 3 of the present note we show that this conjecture is realized to some extent by the formulae derived in ref. 1, which are valid up to first order in the ground state correlations. In section 4 we show quite generally that the spurious states may be discarded from the sums over intermediate states, provided the collective degrees of freedom are treated correctly. In section 2 we review some results of ref. 1 and we derive and correct other results which appear there without derivation.

2 — CORRECTIONS TO RPA TRANSITION AMPLITUDES

In the notation of FUKUDA *et al.* (4), the RPA equations are written as follows

$$(\omega_r + \varepsilon_i - \varepsilon_k)\,\Psi^{(r)}_{ik} = \Theta\,(i\,k) \sum_{jl} \hat{v}_{ij,kl}\,\Psi^{(r)}_{lj} \tag{2.1}$$

where

$$\hat{v}_{ij,kl} = v_{ij,kl} - v_{ij,lk} \tag{2.2}$$

is the antisymmetrized matrix element of the two-body effective interaction, the ε_i are the Hartree-Fock single particle energies and $\Theta\,(i\,k) = -\Theta\,(ki)$ may have the values 1, 0, -1. It is 1 if i is a hole and k is a particle. The eigensolutions of eq. (2.1) can be chosen to satisfy the following orthogonality and completeness relations, when ω_r and ω_s are positive,

$$\sum_{ik} \Psi^{(r)}_{ik}\,\Psi^{(s)*}_{ik}\,\Theta\,(i\,k) = \delta_{rs} \tag{2.3}$$

$$\sum_{ik} \Psi^{(r)}_{ik}\,\Psi^{(s)}_{ki}\;\;\Theta\,(i\,k) = 0 \tag{2.4}$$

$$\sum_r (\Psi^{(r)}_{ik}\,\Psi^{(r)*}_{jl} - \Psi^{(r)*}_{ki}\,\Psi^{(r)}_{lj}) = \delta_{ij}\,\delta_{kl}\,\Theta\,(i\,k) \tag{2.5}$$

In the following we will denote hole states by greek letters, $\alpha, \beta, \gamma, \delta, \ldots$, and we will use the latin letters $m, n, p, q, \ldots$, as indices for particle states. The latin letters $i, j, k, l, \ldots$, may denote either hole or particle states. If we represent by c_i the anihilation operator for the single particle state i, and if the symbol $| >$ stands for the absolute vacuum, the Hartree-Fack ground state is given by

$$| \Phi_o > = \prod_{\alpha} c_{\alpha}^{+} | > \tag{2.6}$$

and the RPA groundstate may be written

$$| 0_{RPA}) \simeq \left(1 + \frac{1}{2} \sum_{m n \alpha \beta} \mathscr{C}_{m \alpha n \beta} c_m^{+} c_{\alpha} c_n^{+} c_{\beta} \right) | \Phi_o > \tag{2.7}$$

where

$$\mathscr{C}_{m \alpha n \beta} \simeq \sum_{s} \Psi_{\alpha m}^{(s)\,*} \Psi_{n \beta}^{(s)} \tag{2.8}$$

In the RPA the matrix element of the operator $c_k^{+} c_i$ between the ground state $| 0)$ and the excited state $| r)$ is given by

$$(r | c_k^{+} c_i | 0)_{RPA} = \Psi_{i k}^{(r)} \tag{2.9}$$

$$(r | c_k^{+} c_i | 0)_{RPA} =$$

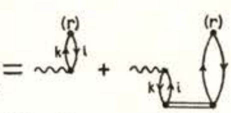

Fig. 1

This expression for the transition amplitude corresponds to the first two diagrams of fig. 1. The contribution of the diagrams of fig. 2 provides the following correction to eq. (2.9)

$$\Delta (r | c_k^{+} c_i | 0) = - \sum_{g h} \left(\Psi_{g h}^{(r)} \Xi_{g i ; h k} + \frac{1}{2} \Psi_{i h}^{(r)} \Xi_{k g ; h g} + \frac{1}{2} \Psi_{h k}^{(r)} \Xi_{h g ; i g} \right) \tag{2.10}$$

$$\Delta (r | c_k^{+} c_i | 0) =$$

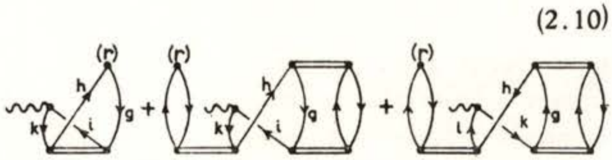

Fig. 2

where

$$\Xi_{ik;jl} = \frac{1}{2}(1 - \Theta(ik)) \sum_s \Psi^{(s)*}_{ik} \Psi^{(s)}_{jl} + \\ + \frac{1}{2}(1 + \Theta(ik)) \sum_s \Psi^{(s)}_{ki} \Psi^{(s)*}_{lj} \tag{2.11}$$

is a small quantity, at most of the order of the small amplitudes $\Psi^{(s)}_{m\alpha}$.

A proof of eq. (2.9) based on the Green function method is presented in ref. 1. An equivalent but simpler derivation of the same equation based on the two-particle-two hole structure of the RPA ground state as given by eq. (2.7) may be found in ref. 2 where the origin of the (1/2) factors is explained.

In the RPA the quantity $(r \mid c_k^+ c_i \mid 0)$ is zero if $\Theta(ik)$ is zero. An expression for that matrix element of first order in the ground state correlations is provided by by eq. (5.18) of ref. 1. Since that expression is not quite correct we will rederive it here following the method developed in ref. 2. We consider the diagrams of fig. 3 for the quan-

$$\Delta(r \mid c_\beta^+ c_\alpha \mid 0) =$$

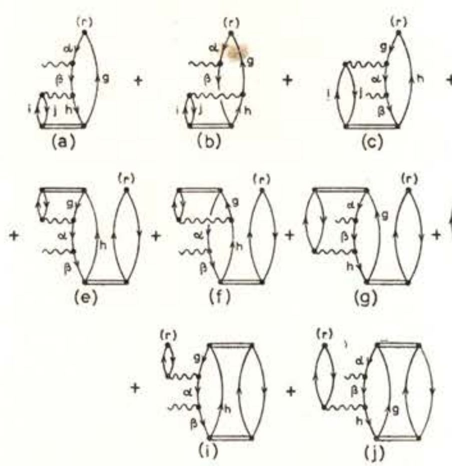

Fig. 3

tity $(r \mid c_\beta^+ c_\alpha \mid 0)$ (or, if we prefer, $\Delta(r \mid c_\beta^+ c_\alpha \mid 0)$ since $(r \mid c_\beta^+ c_\alpha \mid 0)_{RPA}$ is zero). With the conventions of ref. 2, the double-bar in those diagrams represents a factor of the form $\Sigma_s \Psi^{(s)*}_{ik} \Psi^{(s)}_{jl}$ arising from the two-particle-two-hole structure of the RPA ground state. The diagrams (*a*), (*b*), (*c*) and (*d*), which contain only one double-bar, should be the most important ones. The diagrams (*a*) and (*b*) arise from a perturbation theory treatment of the admixture of one-phonon states into the ground state due to ground state correlations. This leads to a correction to the RPA transition amplitude $(r \mid D \mid 0)_{\mathrm{RPA}}$ of the form

$$\Delta' (r \mid D \mid 0) = \sum_t \frac{(r \mid D \mid t)(t \mid H \mid 0)}{E_o - E_t} \tag{2.12}$$

In order to demonstrate in the next section the cancellation of the contributions of spurious states to sums like the one over s contained in the quantity $\overline{\Xi}_{ik;jl}$ which appears in eq. (2.10) it is convenient to leave one half of the contribution of the diagrams (*a*) and (*b*) in the form of eq. (2.12) and to transform the other half as follows. For half the contribution of the diagram (*a*) we may write

$$\Delta_a (r \mid c_\beta^+ c_\alpha \mid 0) = \frac{1}{2} \sum_{ijghs} \frac{\Psi^{(r)}_{\alpha g} \hat{v}_{jh,i\beta} \Psi^{(s)\,\star}_{ji} \Psi^{(s)}_{gh}}{-(\varepsilon_g - \varepsilon_\beta + \Delta)} \tag{2.13}$$

The intermediate state t of eq. (2.12) is here the particle-hole state, containing a particle g, a hole β and having an excitation energy equal to $(\varepsilon_g - \varepsilon_\beta + \Delta)$. The energy shift Δ is introduced in order to account roughly for the particle-hole interaction energy. Now we note that $\Psi^{(s)}_{gh}$ is a small quantity and eq. (2.1) suggests that its most important values are assumed when g and h are such that $-\omega_s \simeq \varepsilon_g - \varepsilon_h + \Delta$. Here, the quantity Δ is possibly about the same as previously. We now introduce a quantity $\mathcal{S}^{(s)}_{ij}$ defined by

$$\begin{aligned} \mathcal{S}^{(s)}_{i} &= \frac{1}{\omega_s + \varepsilon_i - \varepsilon_j} \sum_{kl} \hat{v}_{ik,jl} \Psi^{(s)}_{lj} \quad \text{if} \qquad \Theta(ij) = 0 \\ \mathcal{S}^{(s)}_{ij} &= 0 \quad \text{if} \quad \Theta(if) \neq 0 \end{aligned} \tag{2.14}$$

Then we can write for half the contribution of diagram (*a*)

$$\begin{aligned} \Delta_a (r \mid c_\beta^+ c_\alpha \mid 0) &\simeq \frac{1}{2} \sum_{ghijs} \frac{\Psi^{(r)}_{\alpha g} \hat{v}_{jh,i\beta} \Psi^{(s)\,\star}_{ji} \Psi^{(s)}_{gh}}{\omega_s + \varepsilon_\beta - \varepsilon_h} \\ &\simeq \frac{1}{2} \sum_{ghs} \Psi^{(r)}_{\alpha g} \mathcal{S}^{(s)\,\star}_{\beta h} \Psi^{(s)}_{gh} \end{aligned} \tag{2.15}$$

For half the contribution of diagram (*b*) we obtain in a similar way

$$\Delta_b (r \mid c_\beta^+ \, c_\alpha \mid 0) \simeq - \frac{1}{2} \sum_{ghijs} \frac{\Psi^{(r)}_{\alpha g} \, \hat{v}_{gj,hi} \, \Psi^{(s)*}_{ji} \, \Psi^{(s)}_{h\beta}}{-(\varepsilon_g - \varepsilon_\beta + \Delta)}$$

$$\simeq - \frac{1}{2} \sum_{ghijs} \frac{\Psi^{(r)}_{\alpha g} \, \hat{v}_{gj,hi} \, \Psi^{(s)*}_{ji} \, \Psi^{(s)}_{h\beta}}{\omega_s + \varepsilon_h - \varepsilon_g} \qquad (2.16)$$

$$\simeq - \frac{1}{2} \sum_{ghs} \Psi^{(r)}_{\alpha g} \, S^{(s)*}_{hg} \, \Psi^{(s)}_{h\beta}$$

since, presumably, the most significant values of the small quantity $\Psi^{(s)}_{h\beta}$ are assumed when β and h are such that $-\omega_s \simeq \varepsilon_h - \varepsilon_\beta + \Delta$.

The admixture of two-phonon states into one-phonon states gives rise to a correction to the RPA transition amplitude $(r \mid D \mid 0)_{\mathrm{RPA}}$ of the form

$$\Delta'' (r \mid D \mid 0) = \sum_{st} \frac{(r \mid H \mid st)\,(st \mid D \mid 0)}{E_r - E_s - E_t} \,. \qquad (2.17)$$

Diagrams (*c*) and (*d*) of fig. **3** take this effect into account. The contribution of diagram (*c*) may be written

$$\Delta_c (r \mid c_\beta^+ \, c_\alpha \mid 0) \simeq \sum_{ijgh} \frac{\Psi^{(r)}_{gh} \, \hat{v}_{j\alpha,ig} \, \Psi^{(s)}_{h\beta} \, \Psi^{(s)*}_{ji}}{\omega_r - \omega_s - (\varepsilon_h - \varepsilon_\alpha + \Delta)} \qquad (2.18)$$

where $(\varepsilon_h - \varepsilon_\alpha + \Delta)$ is the energy of phonon t consisting of a hole α and a particle h. We assume that we may write approximately $\omega_r \simeq \varepsilon_h - \varepsilon_g + \Delta$, if h, g are the labels for which $\Psi^{(r)}_{gh}$ is most important. Then we have

$$\Delta_c (r \mid c_\beta^+ \, c_\alpha \mid 0) \simeq \sum_{ijghs} \frac{\Psi^{(r)}_{gh} \, \hat{v}_{j\alpha,ig} \, \Psi^{(s)}_{h\beta} \, \Psi^{(s)*}_{ji}}{-(\omega_s + \varepsilon_g - \varepsilon_\alpha)} \qquad (2.19)$$

$$\simeq - \sum_{gh} \Psi^{(r)}_{gh} \, S^{(s)*}_{g\alpha} \, \Psi^{(s)}_{h\beta}$$

As for diagram (d) we obtain in a similar way

$$\Delta_d(r \mid c_\beta^+ c_\alpha \mid 0) \simeq - \sum_{ghijs} \frac{\Psi_{\alpha g}^{(r)} \hat{v}_{gj,gi} \Psi_{ji}^{(s)\star} \Psi_{h\beta}^{(s)}}{\omega_r - \omega_s - (\varepsilon_h - \varepsilon_\alpha + \Delta)}$$

$$\simeq - \sum_{ghijs} \frac{\Psi_{\alpha g}^{(r)} \hat{v}_{gj,hi} \Psi_{ji}^{(s)\star} \Psi_{h\beta}^{(s)}}{-\omega_s + \varepsilon_g - \varepsilon_h} \tag{2.20}$$

$$\simeq - \sum_{ghs} \Psi_{\alpha g}^{(r)} S_{gh}^{(s)\star} \Psi_{h\beta}^{(s)}$$

where we have assumed

$$\omega_r \simeq \varepsilon_g - \varepsilon_\alpha + \Delta .$$

Notice that diagram (d) is partially canceled by diagram (b). The contribution of the four diagrams (a), (b), (c) and (d), which should be the most important ones, is

$$\Delta_{abcd}(r \mid c_\beta^+ c_\alpha \mid 0) =$$

$$= \sum_{ghs} \left[\frac{1}{2} (\Psi_{\alpha g}^{(r)} S_{\beta h}^{(s)\star} \Psi_{gh}^{(s)} + \Psi_{\alpha g}^{(r)} S_{hg}^{(s)\star} \Psi_{h\beta}^{(s)}) - \right. \tag{2.21}$$

$$\left. - \Psi_{gh}^{(s)} S_{g\alpha}^{(s)\star} \Psi_{h\beta} \right] + \frac{1}{2} \sum_t (r \mid c_\beta^+ c_\alpha \mid t)\, a^{(t)}$$

where (3)

$$(r \mid c_i^+ c_j \mid s) \simeq \sum_k (\Psi_{jk}^{(r)} \Psi_{ik}^{(s)\star} + \Psi_{ki}^{(r)} \Psi_{kj}^{(s)\star}) \qquad \underset{(\text{when } \Theta(ij) = 0)}{\Theta(kj)} \tag{2.21-a}$$

$$a^{(t)} = - \frac{1}{\omega_t} (t \mid H \mid 0)$$

$$\simeq \frac{1}{\omega_t} \sum \Psi_{\beta g}^{(t)} \Psi_{ji}^{(s)\star} (\hat{v}_{jh,i\beta} \Psi_{gh}^{(s)} - \hat{v}_{jg,ih} \Psi_{h\beta}^{(s)}) \tag{2.21-b}$$

the sum being over repeated indices. The quantities $a^{(t)}$ are small, of the order of magnitude of $(\Psi_{m\alpha}^{(t)})^2$, and have the following interpretation. They correspond to the one-phonon components we must add to the

RPA vacuum as given by eq. (2.7) in order to achieve stability against admixture with one-phonon states (3).

For completeness we give now the contribution of all the diagrams of fig. 3.

$$\Delta\,(r\,|\,c_\beta^+\,c_\alpha\,|\,0) \simeq \sum_{g\,h\,s}\Big[\frac{1}{2}(\Psi^{(r)}_{\alpha\,g}\,\Psi^{(s)}_{g\,h}\,S^{(s)\,\star}_{\beta\,h} + \Psi^{(r)}_{\alpha\,g}\,S^{(s)\,\star}_{h\,g}\,\Psi^{(s)}_{h\,\beta}) -$$

$$- S^{(s)\,\star}_{g\,\alpha}\,\Psi^{(r)}_{g\,h}\,\Psi^{(s)}_{h\,\beta} + \frac{1}{2}(S^{(s)}_{\alpha\,g}\,\Psi^{(s)\,\star}_{h\,g}\,\Psi^{(r)}_{h\,\beta} + \Psi^{(s)\,\star}_{g\,\alpha}\,S^{(s)}_{g\,h}\,\Psi^{(r)}_{h\,\beta}) -$$

$$- \Psi^{(s)\,\star}_{g\,\alpha}\,\Psi^{(r)}_{g\,h}\,S^{(s)}_{h\,\beta} + S^{(r)}_{\alpha\,g}\,\Psi^{(s)\,\star}_{h\,g}\,\Psi^{(s)}_{h\,\beta} - \Psi^{(s)\,\star}_{g\,\alpha}\,\Psi^{(s)}_{g\,h}\,S^{(r)}_{h\,\beta}\Big] + \qquad (2.22)$$

$$+ \frac{1}{2}\sum_t\,((r\,|\,c_\beta^+\,c_\alpha\,|\,t)\,a^{(t)} + a^{(t)\,\star}\,(r\,t\,|\,c_\beta^+\,c_\alpha\,|\,0)).$$

$$\Delta(r\,|\,c_m^+\,c_n\,|\,0) =$$

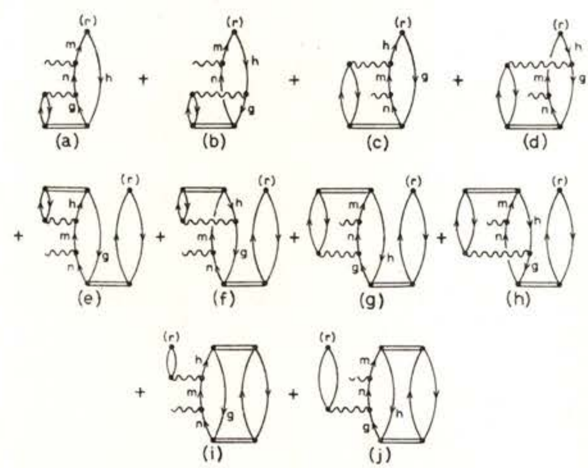

Fig. 4

The contribution of diagrams (a), (b), (c) and (d) of fig. 4, which are there the most important ones, comes out, after analogous manipulations,

$$\Delta_{a\,b\,c\,d}\,(r\,|\,c_m^+\,c_n\,|\,0) \simeq \sum_{g\,h\,s}\Big[\frac{1}{2}(\Psi^{(r)}_{h\,m}\,S^{(s)\,\star}_{g\,n}\,\Psi^{(s)}_{g\,h} +$$

$$+ \Psi^{(r)}_{h\,m}\,S^{(s)\,\star}_{h\,g}\,\Psi^{(s)}_{n\,g}) - \Psi^{(r)}_{g\,h}\,S^{(s)\,\star}_{m\,h}\,\Psi^{(s)}_{n\,g}\Big] + \frac{1}{2}\sum_t\,(r\,|\,c_m^+\,c_n\,|\,t)\,a^{(t)} \qquad (2.23)$$

and the contribution of all the diagrams of fig. 4 is

$$\begin{aligned}\Delta(r\,|\,c_m^+ c_n\,|\,0) \simeq \sum_{ghs}\Big[&\frac{1}{2}(\Psi_{hm}^{(r)} S_{gn}^{(s)*}\Psi_{gh}^{(s)} + \Psi_{hm}^{(r)} S_{hg}^{(s)*}\Psi_{ng}^{(s)}) - \\ &-\Psi_{gh}^{(r)} S_{mh}^{(s)*}\Psi_{ng}^{(s)} + \frac{1}{2}(\Psi_{ng}^{(r)}\Psi_{hg}^{(s)*} S_{hm}^{(s)} + \Psi_{ng}^{(r)} S_{gh}^{(s)}\Psi_{mh}^{(s)*}) - \\ &- S_{ng}^{(s)}\Psi_{gh}^{(r)}\Psi_{mh}^{(s)*} + \Psi_{ng}^{(s)}\Psi_{hg}^{(s)*} S_{hm}^{(r)} - S_{ng}^{(r)}\Psi_{gh}^{(s)}\Psi_{mh}^{(s)*}\Big] + \\ &+\frac{1}{2}\sum_t[(r\,|\,c_m^+ c_n\,|\,t)\,a^{(t)} + (r\,t\,|\,c_m^+ c_n\,|\,0)\,a^{(t)*}]\end{aligned} \tag{2.24}$$

We observe that eqs. (2.22) and (2.24) replace eq. (5.19) of ref. 1, where the terms in $a^{(t)}$ are missing and also some of the remaining terms are incorrect.

$$(rs\,|\,c_i^+ c_k\,|\,0)_{\Theta(ik)=0} =$$

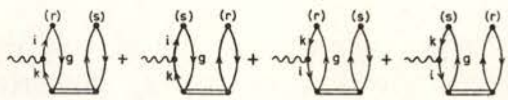

Fig. 5

The two-particle-two-hole structure of the RPA ground state enables the direct excitation of two-phonon states. This effect is represented in fig. 5 and is accounted for by eq. (4.5) of ref. 1 which we quote now

$$(r\,s\,|\,c_i^+ c_k\,|\,0) = \sum_g(\Psi_{kg}^{(r)}\Psi_{gi}^{(s)} + \Psi_{kg}^{(s)}\Psi_{gi}^{(r)}) \qquad \Theta(g\,i) \quad (\text{if } \Theta\; i\,k) = 0) \tag{2.25}$$

A derivation of the same equation in line with our present approach, has been given in ref. 2. Contributions to $(r\,s\,|\,c_i^+ c_k\,|\,0)$ when $\Theta(i\,k) \neq 0$ arise from the admixture of one-phonon states into two-phonon states. This effect contributes a term of the form

$$\Delta(r\,s\,|\,D\,|\,0) = \sum_t \frac{(r\,s\,|\,H\,|\,t)\,(t\,|\,D\,|\,0)}{E_r + E_s - E_t} \tag{2.26}$$

to the transition amplitude $(r\,s\,|\,D\,|\,0)$. The final result may be written as follows

$$\Delta\,(r\,s\,|\,c_i^+\,c_k\,|\,0) \simeq$$
$$\simeq \sum_g \left(\Psi_i^{(r)}\,\mathcal{S}_{gk}^{(s)} + \Psi_{ig}^{(s)}\,\mathcal{S}_{gk}^{(r)} - \mathcal{S}_{ig}^{(r)}\,\Psi_{gk}^{(s)} - \mathcal{S}_{ig}^{(s)}\,\Psi_{gk}^{(r)}\right) \tag{2.27}$$
$$(\text{if } \Theta\,(i\,k) = 0)$$

This equation has been derived in ref. 1. In ref. 2 a derivation, based on diagrams similar to those of fig. 6, has been given for a slightly different version of the same equation.

$$(rs\,|\,c_i^+\,c_k\,|\,0)_{\theta(ik)\neq 0} =$$

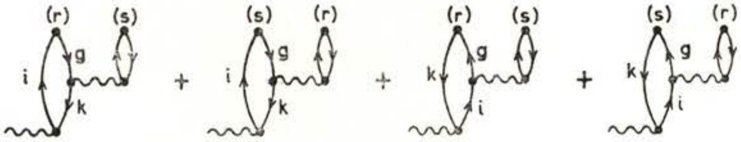

Fig. 6

3 — THE TREATMENT OF SPURIOUS STATES IN EXPRESSIONS OF FIRST ORDER IN THE GROUND STATE CORRELATIONS

Corrections to RPA transition amplitudes which take into account eq. (2.10) but neglect eqs. (2.20) and (2.24) were calculated in ref. 2. In the calculation of correlation corrections to electromagnetic transition amplitudes the terms of eq. (2.10) containing a factor $\frac{1}{2}$ were not taken into account. However, the effect of the omission of the spurious states from the sum over s in eq. (2.11) was considered and it was found to make considerable difference to the transition amplitude. This does not seem correct since the spurious states are generated by collective operators (center of mass position and momentum, etc.), which should commute with boson operators generating intrinsic excitations. It will be shown presently that this situation should be greatly remedied by the inclusion of the terms in eq. (2.10) which contain the factor $\frac{1}{2}$, as has been done in the calculation of form factors for electron scattering. Of course, one should also consider eqs. (2.21) and (2.23).

If we consider an operator

$$D = \sum_{ij} d_{i,j}\, c_i^+ c_j \tag{3.1}$$

eqs. (2.8), (2.9), (2.21) and (2.23) enable us to write

$$(r \mid D \mid 0) = (r \mid D \mid 0)_{RPA} + \Delta (r \mid D \mid 0) \tag{3.2}$$

with

$$(r \mid D \mid 0)_{RPA} = \Sigma\, \Psi_{ij}^{(r)} d_{j,i} \tag{3.3}$$

$$\begin{aligned}\Delta (r \mid D \mid 0) = & -\frac{1}{2} \Sigma \, [\Psi_{\alpha m}^{(r)} \Psi_{m\beta}^{(s)} (\Psi_{n\beta}^{(s)*} d_{n,\alpha} - \\ & - S_{\gamma\beta}^{(s)*} d_{\gamma,\alpha} + \Psi_{\alpha n}^{(s)*} d_{\beta,n} + S_{\alpha\gamma}^{(s)*} d_{\beta,\gamma}) + \\ & + \Psi_{\alpha m}^{(r)} \Psi_{n\alpha}^{(s)} (\Psi_{n\beta}^{(s)*} d_{m,\beta} - d_{m,p} S_{np}^{(s)*} + \Psi_{\beta m}^{(s)*} d_{\beta,n} + \\ & + S_{pm}^{(s)*} d_{p,n}) + \Psi_{\alpha m}^{(r)} S_{\alpha\gamma}^{(s)*} (d_{\beta,\gamma} \Psi_{m\beta}^{(s)} - d_{m,n} \Psi_{n\gamma}^{(s)}) + \\ & + \Psi_{\alpha m}^{(r)} S_{pm}^{(s)*} (d_{p,n} \Psi_{n\alpha}^{(s)} - d_{\beta,\alpha} \Psi_{p\beta}^{(s)})] + \frac{1}{2} \sum_t (r \mid D \mid t)\, a^{(t)}\end{aligned} \tag{3.4}$$

where the summations extend over all repeated indices.

We will assume now that our eq. (2.1) for the RPA is based on the intrinsic part of the hamiltonian in the sense of VILLARS (5). Then the zero energy solutions (spurious states) are doubly degenerate and may be normalized to ∓ 1. We keep the solution with positive norm. A zero energy solution is related to some collective operator $A = \Sigma_{ij}\, a_{i,j}\, c_i^+ c_j$ which commutes with the intrinsic part o the hamiltonian. One may write

$$\Psi_{ik}^{(\text{spurious})} = \theta\,(i\,k)\, a_{i,k} \tag{3.5}$$

$$S_{ik}^{(\text{spurious})} = \frac{1}{\varepsilon_i - \varepsilon_k} \sum_{jl} \hat{v}_{ij,kl}\, \Psi_{lj}^{(\text{spurious})} = a_{i,k} \tag{3.6}$$

These equations follow from the commutation relations of A with the intrinsic part of the hamiltonian. If D commutes with A it is seen that the spurious states nearly cancel out in the sum over s in eq. (3.4). Apparently a term of the form

$$
\begin{aligned}
&-\frac{1}{2}\,\Sigma\,[\Psi^{(r)}_{\alpha m}\,\mathcal{S}^{(s)\,*}_{\alpha\gamma}\,(d_{m,\beta}\,\mathcal{S}^{(s)}_{\beta\gamma}-\mathcal{S}^{(s)}_{mn}\,d_{n,\gamma})\,+ \\
&+\Psi^{(r)}_{\alpha m}\,\mathcal{S}^{(s)\,*}_{pm}\,(\mathcal{S}^{(s)}_{pn}\,d_{n,\alpha}-d_{p,\gamma}\,\mathcal{S}^{(s)}_{\gamma\alpha})]
\end{aligned}
\qquad (3.7)
$$

is still needed in eq. (3.4) in order for the contribution of the spurious states to cancel out exactly. However, such a term would correspond to diagrams like those shown in fig. 7 and is of higher

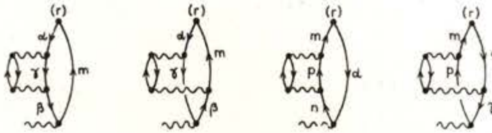

Fig. 7

order (second order perturbation theory in the phonon-phonon interaction). It is therefore reasonable to omit the spurious states in the sums over s in eq. (3.4), since it seems possible to cause the contribution of the spurious states to cancel out in that equation by introducing appropriate higher order terms which otherwise (as far as the remaining states are concerned) should be unimportant. The fact that the spurious states do not cancel out exactly in our approximation (it being necessary for that to introduce also some terms which may be considered of higher order) is due to the fact that our spurious states are not 100 % spurious. It should be possible to reformulate the theory in such a way as to treat correctly to the desired order the collective degress of freedom. Then one would deal with truly spurious states which, as a whole, would have an exactly zero contribution. However, that kind of approach should not lead to essentialy new results and does not seem convenient for practical computations. The term in expression (3.7) corresponding to a spurious s state measures our error in neglecting the spurious states. The sum over t in eq. (3.4) should be assumed to extend only over non spurious states, since the quantity $a^{(t)}$ should be zero for spurious states. Indeed, the $a^{(t)}$ are the amplitudes of the one-phonon components we must add to the RPA ground state in order to achieve stability against admixture with one-phonon states. If H is the intrinsic hamiltonian, in VILLARS sense (5), the RPA ground state is automatically stable against admixture with spurious states so that one expects $a^{(t)}$ to be zero when $|t)$ is a spurious state.

We discuss now the transition amplitude to a two-phonon state, when one of the phonons is spurious. If, for instance, the state s is a spurious state, one would expect the quantity $(rs|D|O)$ to cancel out, since D is an intrinsic operator and the state $|s)$ is generated by a collective operator which commutes with D. However our spurious states are not 100 % spurious, so it is appropriate to try and find out to what extend this conjecture is realized. The matrix element $(rs|D|O)$ may be calculated with the help of eqs. (2.25) and (2.27). Keeping only the larger terms, which contain at least one large amplitude $\Psi^{(r)}_{\alpha m}$ or $\Psi^{(s)}_{\alpha m}$ we find

$$
\begin{aligned}
(rs|D|0) \simeq \Sigma\, [\Psi^{(r)}_{\alpha m} (d_{m,n}\,\Psi^{(s)}_{n\alpha} - d_{m,\beta}\,\mathcal{S}^{(s)}_{\beta\alpha} - \\
- \Psi^{(s)}_{m\beta}\, d_{\beta,\alpha} + \mathcal{S}^{(s)}_{mn}\, d_{n,\alpha}) + \Psi^{(s)}_{\alpha m} (d_{m,n}\,\Psi^{(r)}_{n\alpha} - \\
- d_{m,\beta}\,\mathcal{S}^{(r)}_{\beta\alpha} - \Psi^{(r)}_{m\beta}\, d_{\beta,\alpha} + \mathcal{S}^{(r)}_{mn}\, d_{n,\alpha})]
\end{aligned}
\qquad (3.8)
$$

the sum being over all repeated indices. If s is a spurious state s_o and D is an intrinsic operator (which commutes with the previously considered operator A) then eq. (3.8) becomes simply

$$
(r s_o|D|0) \simeq \Sigma\, \Psi^{(s_o)}_{\alpha m} (d_{m,n}\,\Psi^{(r)}_{n\alpha} - d_{m,\beta}\,\mathcal{S}^{(r)}_{\beta\alpha} - \Psi^{(r)}_{m\beta}\, d_{\beta,\alpha} + \mathcal{S}^{(r)}_{mn}\, d_{n,\alpha})
$$

In general the state r is not strongly collective, so that the amplitudes $\Psi^{(r)}_{n\alpha}$ and $\mathcal{S}^{(r)}_{ij}$ are small quantities and the magnitude of $(r s_o|D|0)$ is negligible in the average. If it does not come out exactly zero it is only because our spurious states are not exactly spurious. They are generated by operators A which are only approximately collective.

4 — GENERAL TREATMENT OF THE SPURIOUS STATES

We will now show, under rather general arguments, that the contribution of the spurious states actually cancels out and should be discarded from expressions of the type we have been considering. In order to tackle this problem we introduce the projection operator of the vacuum $|0\}$ of the boson operators B_μ. From the commutation relations

$$[B_\mu, B_\nu] = [B_\mu^+ B_\nu^+] = 0 \qquad [B_\mu, B_\nu^+] = \delta_{\mu\nu} \tag{4.1}$$

It follows that the projection operator Q of the vacuum $|0\}$ may be written (6)

$$Q \equiv |0\}\{0| = 1 - \sum_\mu B_\mu^+ B_\mu + \frac{1}{2!}\sum_{\mu\nu} B_\mu^+ B_\nu^+ B_\nu B_\mu - \frac{1}{3!}\sum_{\mu\nu\sigma} B_\mu^+ B_\nu^+ B_\sigma^+ B_\sigma B_\nu B_\mu + \ldots \tag{4.2}$$

one readily verifies the results

$$Q^2 = Q \tag{4.3}$$

$$Q|0\} = |0\} \tag{4.4}$$

$$Q B_\mu^+ |0\} = Q B_\mu^+ B_\nu^+ |0\} = \ldots = 0 \tag{4.5}$$

it is also interesting to consider the operators

$$q_\mu = 1 - B_\mu^+ B_\mu + \frac{1}{2!} B_\mu^{+2} B_\mu^2 - \frac{1}{3!} B_\mu^{+3} B_\mu^3 + \ldots, \tag{4.6}$$

$$Q_{\alpha\beta\ldots\gamma} = 1 - \sum_{\mu \neq \alpha\beta\ldots\gamma} B_\mu^+ B_\mu \frac{1}{2!} \sum_{\substack{\mu \neq \alpha\beta\ldots\gamma \\ \nu \neq \alpha\beta\ldots\gamma}} B_\mu^+ B_\nu^+ B_\nu B_\mu - \ldots \tag{4.7}$$

The operator q_μ projects on to the states which do not contain the phonon μ while the operator $Q_{\alpha\beta\ldots\gamma}$ projects on to the vacuum or the states which contain only phonons $\alpha\beta\ldots\gamma$.

Obviously

$$Q = \prod_\mu q_\mu \tag{4.8}$$

$$Q_{\alpha\beta\ldots\gamma} = \prod_{\mu \neq \alpha\beta\ldots\gamma} q_\mu \tag{4.9}$$

In order to calculate the expectation value of an operator A in the boson vacuum $|0\}$ we consider the identity

$$\}0|A|0\{ = \frac{<\Phi_o|QAQ|\Phi_o>}{<\Phi_o|Q|\Phi_o>}, \tag{4.10}$$

which, on account of eq. (4.2), leads immediately to an expansion for $\}0|A|0\{$ in sums over boson states μ (the first term in that expansion is $<\Phi_o|A|\Phi_o>$, the next term is given as a single sum over μ etc.).

The operator A may be, for instance, the commutator $[B_\mu, M]$, where M is a transition operator, or A may be the mean square radius operator, etc. From symmetry considerations we may know, *a priori*, that A commutes with some boson operators, say, those corresponding to the indices $\alpha\beta\ldots\gamma$. For instance, if A is the intrinsic part of the hamiltonian, or of any other operator, as discussed by Villars (5) it commutes with the momentum and center of mass operators. (Then the operators $B_\alpha, \ldots, B_\gamma, B_\alpha^+, \ldots, B_\gamma^+$, would be some linear combinations of the momentum and center of mass operators, assuming a spherical system). We want to show that under such circumstances we may werite

$$\}0|A|0\{ = \frac{<\Phi_o|Q_{\alpha\beta\ldots\gamma}AQ_{\alpha\beta\ldots\gamma}|\Phi_o>}{<\Phi^o|Q_{\alpha\beta\ldots\gamma}|\Phi_o>} \tag{4.11}$$

thus effectively dropping out, from the sums over intermediate states, the terms containing the labels $\alpha\beta\ldots\gamma$ (the spurious states). This result becomes obvious if we remark that

$$Q_{\alpha\beta\ldots\gamma} = \sum_{n_\alpha\, n_\beta \ldots n_\gamma} | n_\alpha\, n_\beta \ldots n_\gamma \} \frac{1}{n_\alpha!\, n_\beta! \ldots n_\gamma!} \{ n_\alpha\, n_\beta \ldots n_\gamma | \qquad (4.12)$$

where $n_\alpha \ldots n_\gamma$ designate the numbers of the phonons $\alpha \ldots \gamma$. One also has

$$\begin{aligned} &\{ n_\alpha\, n_\beta \ldots n_\gamma | A | n'_\alpha\, n'_\beta \ldots n'_\gamma \} \\ &\quad = \{ 0 | A | 0 \}\, n_\alpha!\, n_\beta! \ldots n_\gamma!\, \delta_{n_\alpha n'_\alpha}\, \delta_{n_\beta n'_\beta} \ldots \delta_{n_\gamma n'_\gamma} \end{aligned} \qquad (4.13)$$

Therefore we see that

$$\begin{aligned} &< \Phi_o | Q_{\alpha\beta\ldots\gamma}\, A\, Q_{\alpha\beta\ldots\gamma} | \Phi_o > \\ &= \{0|A|0\} \sum_{n_\alpha\, n_\beta \ldots n_\gamma} < \Phi_o | (| n_\alpha\, n_\beta \ldots n_\gamma \} \frac{1}{n_\alpha!\, n_\beta! \ldots n_\gamma!} \{ n_\alpha\, n_\beta \ldots n_\gamma |) | \Phi_o > \\ &= \{ 0 | A | 0 \} < \Phi_o | Q_{\alpha\beta\ldots\gamma} | \Phi_o > \end{aligned}$$

which proves eq. (5.10).

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