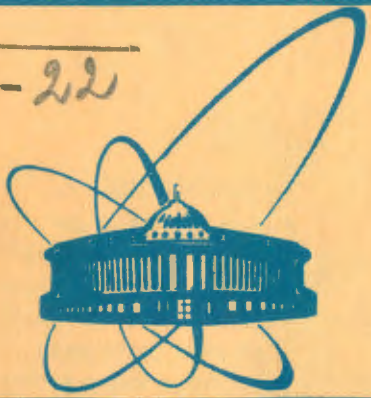

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RESONANT STATES IN STRUCTURE CALCULATIONS

(Continued)

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1. Introduction

In a recent paper, henceforth referred to as I. [1], it was suggested to introduce resonant states as a means of treating continuum admixtures in nuclear wave functions. Since the calculational problems, connected with finding the resonance poles and the corresponding wave functions have recently been solved [2], we shall here present a number of useful formulae, suited for different types of structure calculations. In this way, the paper appears as a continuation of I.

We shall first discuss the underlying mathematical formalism, and give a number of relations, which serve as a completion of those given in I and in our earlier papers [3,4].

Next, we shall give a description of what could be called a complex decaying state. By this we mean a state, which contains many components of shell model type, i.e., particle-hole states or several-particle - several-hole states, still containing only components with one particle in the continuum and no incoming particles.

This restriction which is common to all calculations of the continuum shell model type seems necessary for mathematical reasons [5]. In the present context, its role is rather obvious, since we build our approach on a Mittag-Leffler expansion of the single particle Green's functions, satisfying the Lipmann-Schwinger equation, whereas a consistent treatment of states with two particles in the continuum must start from the Faddeev equations.

Our states are therefore suited for description of such complex states, which lie above the threshold for emission of one single nucleon only, or where, at least, such an emission is the dominating particle decay mode. Such states could, e.g., be giant resonance states, decaying by emission of neutrons or protons.

Finally we shall look at the one particle strength functions as is seen, e.g., in elastic scattering of neutrons or protons. The calculations of the fragmentation and spreading, shown by such strength functions contain a non-statistical as well as a statistical part. The first one should, at least in principle, be calculable from a microscopic description of nuclear states. Here, however, it is obvious that a description of the continuum wave functions is needed.

We shall discuss an example of strength functions connected with the states of odd nuclei.

2. The expansions in terms of pole funotions

The expansion of arbitrary functions in terms of pole functions is, in contrast to the usual expansions, used in many branches of physics, not unambiguous, as is seen from the overcompleteness of this basis

$$\sum_i \varphi_i(r)\,\varphi_i(r') = 2\,\delta(r-r') \tag{2.1}$$

or from the relation

$$\sum_i \frac{\varphi_i(r)\,\varphi_i(r')}{K_i} = 0. \tag{2.2}$$

Unambigous expansions are nevertheless obtained for a limited range of $r(r')$ values, for the scattering wave funotions and Green's funotions using the fact that the $\varphi_i(r)$'s correspond to residues at the poles of these functions, and that therefore a Mittag-Leffler expansion of G in terms of $\varphi_i(r)\varphi_i(r')$ with the requirement that it contains no entire part, is unique. From this an unambigous expansion of the scattering function $\gamma^{(+)}$ is also obtained. This was, e.g., used to obtain the equations I (3.8), I (3.9) .

A different situation is met, when a truncated set of poles is used. The two expressions

$$G_N^{(+)}(K) = \sum_n^N \frac{\varphi_n(r)\,\varphi_n(r')}{2K_n(K-K_n)} \tag{2.3}$$

and

$$\begin{aligned} G_N^{(+)}(K) &= \sum_n^N \frac{\varphi_n(r)\,\varphi_n(r')}{2K_n(K-K_n)} + \\ &+ C\sum_n^N \frac{\varphi_n(r)\,\varphi_n(r')}{2K_n} = \\ &= \sum_n^N \frac{\varphi_n(r)\,\varphi_n(r')\,(1+C(K-K_n))}{2K_n(K-K_n)} \end{aligned} \tag{2.4}$$

are obviously not equivalent for a finite N-value, although they differ by a K-independent term only.

Here, the second expression, (2.4), obviously has some undesirable properties. Thus, e.g., the usual convergence of the distorted wave Born approximation with large energies, which is due to the denominator of $G^{(+)}(K)$ would not be found with $G_N^{(+)}(K)$. It ought to be mentioned here that only one further problem of

ambiguity is connected with obtaining I (3.20), I (3.21) from I (3.5), I (3.6). Instead of I (3.7) we could obviously, based on I (3.6), write

$$b_{\lambda'}(k') = (K_{\lambda'}^2 - k'^2)^{-1} \int dr\, \gamma_{\lambda'}^{+}(k'r)\, U_\lambda(r) \tag{2.5}$$

(U_λ independent of k').

Then, the third term in I (3.8) and I (3.9) will be, respectively

$$\begin{aligned} &\frac{2}{\pi}\sum_\lambda \langle \lambda'|V_1 \int_0^\infty dk\, \gamma_\lambda^{+}(kr) \frac{1}{K_\lambda^2 - k^2} \int dr'\, \gamma_\lambda^{+}(kr')\, U_\lambda(r')|\lambda\rangle = \\ &= \frac{2}{\pi}\langle \lambda'|V_1 \int dr'\, G_{\lambda\rho}(K_\lambda, r, r')\, U_\lambda(r')|\lambda\rangle \end{aligned} \tag{2.6}$$

and

$$\begin{aligned} &\frac{2}{\pi}\sum_\lambda \langle \varphi_i,\lambda'|V_1 \int_0^\infty dk\, \gamma_\lambda^{+}(kr) \frac{1}{K_\lambda^2 - k^2} \int dr'\, \gamma_\lambda^{+}(kr')\, U_\lambda(r')|\lambda\rangle = \\ &= \frac{2}{\pi}\langle \varphi_i,\lambda'|V_1 \int dr'\, G_{\lambda\rho}(K_\lambda, r, r')\, U_\lambda(r')|\lambda\rangle . \end{aligned} \tag{2.7}$$

Here, if the singular integrals are interpreted by $K_\lambda = K_\lambda + i0$, the G_p of (2.6) and (2.7) is obviously G_p^{+}.

Now, when we introduce the Mittag-Leffler expansion of G_p^{+}

$$G_{\lambda\rho} = \sum_i \frac{\varphi_{i(\lambda)}(r)\,\varphi_{i(\lambda)}(r')}{2K_i(K_\lambda - S_i K_i)} \tag{2.8}$$

$S_i = -\mathrm{sign}\,(\mathrm{Im}(K_i))$

in these expressions, we immediately arrive at the nondiagonal terms of the expressions I (3.19) – I (3.21) with

$$\beta_{i\lambda} = \int dr\, \varphi_{i(\lambda)}(r)\, U_\lambda(r). \tag{2.9}$$

To get the diagonal term, we just notice that from (2.5)

$$(k'^2 - K_{\lambda'}^2)\, b_{\lambda'}(k') = -\int dr\, \gamma_{\lambda'}^{+}(k'r)\, U_{\lambda'}(r) \tag{2.10}$$

must have a pole at $k' = K_i$. Taking the residuum here, we obviously get back the extra diagonal term corresponding to $\beta_{i\lambda'}$ of I (3.9).

In this argumentation we have used a) that the integral in (2.5) is convergent (and therefore, as usual, that the upper limit can be put equal to R), b) that the pole expansion (2.8) of G_p and the similar expansion of $\gamma^{+}(r^c)$ used in (2.10) and I (3.9) determine these funotions, i.e., that no entire function of k or k' is allowed, even when the expansion is truncated . c) In writting I (3.20) we have further assumed that the matrix M has an inverse. Looking apart from accidental degeneracies, this assumption is valid only if the expansion of the total wave function in terms of pole functions

is unambigious . A similar problem is met when no source term is present, and we have to find an eigenvalue, corresponding to a complicated decaying state.

Now, the interdependence of the pole functions, equation (2.2), will of course in principle prevent this uniqueness in the general case.

However, when a final number of poles is used, in the expansion of both the Green's function and the single particle scattering functions, the expansion is in general unique.

The proof runs as follows. If the expansion

$$f_N(z) = \sum_i^N \alpha_i \varphi_i(z) \qquad (z \le R) \tag{2.11}$$

is not unambiguous, there must exist a linear relation between the pole functions

$$\sum_i^N \gamma_i \varphi_i(z) = 0 \qquad (z \le R)\,. \tag{2.12}$$

Applying now the single particle Hamiltonian to (2.12) we get

$$0 = (H_0 + V)\sum_i^N \gamma_i \varphi_i = \sum_i^N \gamma_i \kappa_i^2 \varphi_i\,. \tag{2.13}$$

This procedure can be repeated, to get an overdetermination of the γ's so that only $\gamma_i = 0$, all i, is a solution. Look, e.g., at N = 3

$$\gamma_1 \varphi_1 + \gamma_2 \varphi_2 + \gamma_3 \varphi_3 = 0 \tag{2.14}$$

$$\gamma_1 \kappa_1^2 \varphi_1 + \gamma_2 \kappa_2^2 \varphi_2 + \gamma_3 \kappa_3^2 \varphi_3 = 0$$

gives

$$\gamma_2(\kappa_2^2 - \kappa_1^2)\varphi_2 + \gamma_3(\kappa_3^2 - \kappa_1^2)\varphi_3 = 0 \tag{2.15}$$

operating with $(H_0 + V)$ gives

$$\gamma_2(\kappa_2^2 - \kappa_1^2)\kappa_2^2\varphi_2 + \gamma_3(\kappa_3^2 - \kappa_1^2)\kappa_3^2\varphi_3 = 0 \tag{2.16}$$

from (2.15) and (2.16) we get

$$(\kappa_3^2 - \kappa_1^2)(\kappa_3^2 - \kappa_2^2)\gamma_3\varphi_3 = 0 \tag{2.17}$$

or more generally

$$\prod_{j(\neq i)}^N (\kappa_i^2 - \kappa_j^2)\gamma_i\varphi_i = 0\,. \tag{2.18}$$

Now, as we have shown in ref. /3/ (appendix) the possibility of coincidence of the poles can in general be ignored.

This argument cannot in a convergent way be extended to $N \to \infty$, so no contradiction with (2.2) is found. Still, the appearance in I (3.20), etc., of the same function, φ, both in the expansion of a bound state as φ_ν, and in the pole expansion of γ^G as φ_n, seems to contradict this linear independence. Here, however, we should remember that φ_ν and φ_n go into the calculation of the matrix M in different ways as is seen, e.g., from the fact that even if we write $|\lambda\rangle \equiv |\nu\lambda\rangle$ with $\varphi_\nu = \varphi_n$, we have nevertheless

$$\langle \lambda n | M | \lambda n \rangle \neq \langle \lambda\nu | M | \lambda n \rangle\,, \qquad \text{etc.}$$

The overcompleteness must mean that in a concrete calculation, the matrix inversion of diagonalization will become specially difficult, when the number of pole terms becomes large. It was, however, shown in ref. /4/ that in a realistic situation, corresponding to a nuclear physics potential, a relatively small number of terms was sufficient in the pole expansion of $G^{(+)}$. The convergence of the pole expansion can, by use of the Mittag-Leffler theorem /3,4/ be improved considerably, introducing entire terms in G (and γ^G). It should be noted that by means of the Kapur-Peierls functions also the entire term can for $z, z' \le R$ be written as a sum of separable operators, with a simple polynomial dependence of K.

In I, the theory of shell model-continuum states was developed, and the pole functions introduced, using the Mittag-Leffler expansion of $G^{(+)}$. This means that the singular integrals in I (3.8) and I (3.9) are interpreted in the same way as they are in the definition of $G^{(+)}$. This leads, as mentioned by Bloch /4/, to a particularly simple, linear expression for the scattering matrix by means of what is usually called the $\mathcal{T}$-matrix (Bloch's notation is different).

However, instead of the $\mathcal{T}$-matrix scattering theory is often expressed in terms of the K-matrix, which is obtained in a similar way, only with the singular integrals of the shell-model-continuum theory, our I(3.8), I (3.9), interpreted as principal value integrals. If this is done, the G_ρ of our equations (2.6), (2.7) must be

G^P_P, the continuum part of the principal value Green's function. The pole expansion of G^P is easily obtained from that of G^+. We may, e.g., use equation (2.21) of ref. /3/

$$G^+ = \frac{1}{2}\sum_n \frac{\varphi_n(r)\varphi_n(r')}{K^2-K_n^2} + \frac{K}{K_n}\frac{\varphi_n(r)\varphi_n(r')}{(K^2-K_n^2)} \qquad (2.17)$$

to get

$$G^P = Re(G^+) \quad (K \text{ real}) \qquad (2.18)$$

$$= \frac{1}{2}\sum_n \frac{\varphi_n(r)\varphi_n(r')}{K^2-K_n^2}.$$

So, for the continuum part we get the simple expression

$$G^P_P = \frac{1}{2}\sum_{n\ (\text{all poles})} \frac{\varphi_n(r)\varphi_n(r')}{K^2-K_n^2} - \sum_{n\ (\text{bound states})} \frac{\varphi_n(r)\varphi_n(r')}{K^2-K_n^2} = \qquad (2.19)$$

$$= \frac{1}{2}\sum_{n\ (\text{all poles})} \frac{S_n\varphi_n(r)\varphi_n(r')}{K^2-K_n^2},$$

where, as in I, $S_n = +1$ for poles in the lower half k-plane, $S_n = -1$ in the upper.

The pole expansion of G^P must of course essentially have the same convergence properties as those of G^+. When a truncated set of poles is used, the requirement, that G^P_N should be real leads to the natural exigency that the truncated set, for each resonance pole, must also contain its mirror pole. Note that in this case $\sum_n^N \frac{\varphi_n(r)\varphi_n(r')}{K_n}$ is purely imaginary.

3. Complex decaying states

As mentioned above, we can inside the framework of the present theory only give a precise description of such states, where at most one particle is in the continuum. Of course, a product of two of our states or a sum of such products can, properly antisymmetrized, be interpreted as a state with two particles in the continuum, and so on, but such products are eigenstates of the Hamiltonian only, in the approximation, that some particle-particle coupling terms can be neglected.

So let us look at the continuum shell model equation obtained from I (3.8), I (3.9) in the absence of source terms. Here, in order to obtain a decaying state, we must interpret the singular integrals as in the definition of G^+ and we obtain

$$\underline{\underline{M}}\,\underline{\alpha} = 0, \qquad (3.1)$$

where $\underline{\underline{M}}$ and $\underline{\alpha}$ are given by I (3.21) and I (3.19), respectively.

Alternatively, we can in the random phase approximation get the same expression, with $\underline{\alpha}$ given by I (4.13), I (4. 14) and $\underline{\underline{M}}$ given by I (4.16), I (4.17).

Starting with the first approach, we see that solutions of (3.1) are possible, if

$$Det\left(\underline{\underline{M}}(E)\right) = 0. \qquad (3.2)$$

The solutions obviously have the form given by I (3.2) and I (3.4)

$$|\Psi> = \sum \alpha_\lambda |\lambda> + \frac{2}{\pi}\sum_\lambda \int dk\, b_\lambda(k)|k\lambda>, \qquad (3.3)$$

where b_λ is given in terms of the α's by I (3.7), I (3.19). To discuss the structure of these equations, let us look at the example of only one bound state and one resonance in one channel. Now (3.2) is written

$$\begin{vmatrix} <\lambda|V_I|\lambda> - (k^2+e_\lambda-E_\lambda) & <\lambda|V_I|\tau> & <\lambda|V_I|i> \\ <i|V_I|\lambda> & <i|V_I|\tau> + 2\kappa_i^*(k+\kappa_i^*) & <i|V_I|i> \\ <\tau|V_I|\lambda> & <\tau|V_I|\tau> & <\tau|V_I|i> - 2\kappa_i(k-\kappa_i) \end{vmatrix} = 0. \qquad (3.4)$$

For the sake of simplicity, let us assume the diagonal elements and the pole-pole coupling terms of V_I to be zero. Then we have

$$\frac{V_{I\lambda}^{*2}}{2\kappa_i^*(\kappa_i^*+\kappa)} + \frac{V_{I\lambda}^{2}}{2\kappa_i(\kappa_i-\kappa)} = (E_\lambda - e_\lambda - k^2). \qquad (3.5)$$

It is seen that a purely imaginary k-value corresponding to a bound state solution is generally possible, since in the interval $0 < \varkappa < \infty$ both sides of the equation are real, and the left-hand side will go from $Re\left(\frac{V_{I\lambda}^2}{2\kappa_i^2}\right)$ to 0, but the right-hand side from $E_\lambda - e$ to $+\infty$, where $E - e < 0$, $Re\left(\frac{V_{I\lambda}^2}{2\kappa_i^2}\right) > 0$, $i\varkappa = K$.

Formally, a solution with $\varkappa^2 < 0$ may in general also exist, it should, however, be discarded, since in obtaining (3.1) we used, among other relations, I (3.15), which excludes $\varkappa^2 < 0$. It is also seen that for a large class of parameters the other roots must be complex (3 real roots must be a rare exoeption). So, as we should expeot, oomplex energies, oorresponding to mixed resonances must result from eq. (3.4), or the general eq. (3.2). For weak couplings we may, in the neighbourhood of a single particle resonance write (3.5) with

$$k = \kappa_i + \alpha$$

$$-\frac{V_{i\lambda}^2}{2\kappa_i \cdot \lambda} + \frac{V_{i\lambda}^{*2}}{2\kappa_i^* (k_i + k_i^*)} \approx E_\lambda - e_\lambda - k_i^2 \qquad (3.6)$$

$$\alpha \approx \frac{V_{i\lambda}^{*2}}{2\kappa_i (\kappa_i + e_\lambda - E)} .$$

The corresponding 1. Order wave function

$$|\psi\rangle = \alpha_\lambda |\lambda\rangle + \alpha_{\tau_1} |\varphi_{\tau_1} \lambda\rangle + \alpha_{\tau_2} |\varphi_{\tau_2} \lambda\rangle \qquad (3.7)$$

is, up to normalization obtained as

$$\psi^{(1)} \approx \frac{V_{i\lambda}}{E_\lambda - e_\lambda - k_i^2} |\lambda\rangle + |\varphi_i \lambda\rangle \qquad (3.8)$$

which is formally identical to the usual 1. Order perturbation expression.

In the Random Phase Approximation, a similar eigenvalue problem, although more oomplioated, is found.

Here, only instead of the elimination of E, $E = \kappa_\lambda^2 + e_\lambda$ above, we have in the different diagonal matrix elements of M (see I (4.17)) to eliminate E , -E and, say, κ_{λ^-} by

$$\kappa_{\lambda^-} = +i\sqrt{|e_\lambda| \cdot 2 + \kappa_{\lambda^+}^2} .$$

Whereas the complex soattering states, as solutions of an inhomogeneous equation, are normalized by the ohoice of the inhomogeneous term, the coefficients in the equation for the complex decaying state should be normalized according to the usual conventions.

So we have, for

$$|\psi\rangle = \sum_\lambda \alpha_\lambda |\lambda\rangle + \frac{2}{\pi} \sum_\lambda \int d\kappa \, f_\lambda(\kappa) |\kappa\lambda\rangle \qquad (3.9)$$

$$\langle\psi|\psi\rangle = \sum_\lambda |\alpha_\lambda|^2 + \frac{2}{\pi} \sum_\lambda \int dk \, |b_\lambda(k)|^2 = 1 \qquad (3.10)$$

now, as above

$$b_\lambda(k) = (k_\lambda^2 - k)^{-1} \int dz \, \gamma_\lambda^{(+)}(k,z) U_\lambda(z) . \qquad (3.11)$$

So the integrals in (3.10) can be written

$$I = \int dk \, (k_\lambda^2 - k^2)^{-1} (k_\lambda^{*2} - k^2)^{-1} \cdot \qquad (3.12)$$

$$\cdot \int dz \, \gamma_\lambda^{(+)}(k,z) U_\lambda(z) \int dz \, \gamma_\lambda^{+*}(kz) U_\lambda^*(z) =$$

$$= \frac{1}{\kappa_\lambda^{*2} - \kappa_\lambda^2} \int dk \, \left((k_\lambda^2 - k^2)^{-1} - (k_\lambda^{*2} - k^2)^{-1} \right) \cdot$$

$$\cdot \iint dz\, dz' \, \gamma_\lambda^+(k,z) \, \gamma_\lambda^{+*}(kz') U_\lambda(z) U_\lambda^*(z')$$

or

$$I = \frac{1}{k_\lambda^{*2} - k_\lambda^2} \frac{\pi}{2} \iint dz\, dz' \left(G_\rho^+(k_\lambda, z, z') - G_\rho^-(k_\lambda^*, z, z') \right) =$$

$$= \frac{1}{k_\lambda^{*2} - k_\lambda^2} \frac{\pi}{2} \iint dz\, dz' \sum_i \left(\frac{1}{2k_i (k_\lambda - s_i k_i)} - \frac{1}{2k_i (-k_\lambda^* - s_i k_i)} \right) \cdot \qquad (3.13)$$

$$\cdot \varphi_i(z) \varphi_i(z') U_\lambda(z) U_\lambda^*(z') =$$

$$= \frac{1}{k_\lambda^2 - k_\lambda^{*2}} \frac{\pi}{2} \sum_i \frac{k_\lambda + k_\lambda^*}{2k_i (k_\lambda - s_i k_i)(-k_\lambda^* - s_i k_i)} \beta_{\tau\lambda} \beta_{i\lambda}^* =$$

$$= \frac{1}{k_\lambda^* - k_\lambda} \frac{\pi}{2} \sum_i 2\kappa_i \alpha_{\tau\lambda}^+ \alpha_{i\lambda}^{+*} .$$

Since $k_{i^-} = -k_i^*$, this expression is purely real, as long as

we still retain the rule, that if the expansion contains i, it must also contain $\tilde{i}$.

The normalization of the corresponding states, obtained in the Random Phase Approximation is given by

$$\sum_{\lambda}\left(|\alpha_{\lambda+}|^2-|\alpha_{\lambda-}|^2\right)+\frac{2}{\Pi}\sum_{\lambda}\int dk\left(|b_{\lambda+}(k)|^2-|b_{\lambda-}(k)|^2\right), \tag{3.14}$$

where $b_{\lambda\pm}$ can be expressed as above, using the $k_{\lambda\pm}$ given in I (4.11).

4. Quasi-particles, strength functions

We shall here discuss particle strength function calculations, using the pole expansion, for a particular example, which contains, however, in principle the main problems, met in the general case.

The example concerns an odd nucleus. We shall here look at the approximate description, relevant, when many particles are outside a closed shell. The even system, obtained by removing the odd particle, is in an approximate eigenstate of a Hamiltonian, which besides the shell model potential contains a short range particle-particle interaction and some interactions of larger range. The correlations introduced by the short range interaction are of the pairing type, and they are treated by introducing the Bogolubov transformation

$$\begin{aligned}\alpha(\nu)^+ &= u_\nu\, a^+(\nu)+v_\nu\, a(\tilde{\nu}),\\ \alpha(\tilde{\nu})^+ &= u_\nu\, a^+(\tilde{\nu})-v_\nu\, a(\nu).\end{aligned} \tag{4.1}$$

Here the continuum states must be completely unoccupied in the even core, so we must have

$$v_\nu = 0 \quad (u_\nu = 1)\ , \quad \varepsilon_\nu > 0\,. \tag{4.2}$$

This means that these states do not enter in the description on equal footing with the bound states, but since v_ν , so far above the Fermi level must anyhow be very small, the pairing picture is not noticeably modified.

The long range interactions are treated in the Random Phase Approximation. This means that from pairs of the quasi-particle operators, $\alpha(\nu)$, etc., given above, new collective boson-like operators are constructed by the transformation

$$Q^{+i}_{\lambda\mu}=\sum_{j(\nu)j'(\nu')}\left(\left[\alpha^+_{jm}(\nu)\alpha^+_{j'm'}(\nu')\right]_{\lambda\mu}\psi^{\lambda i}_{j(\nu)j'(\nu')}+(-1)^{\lambda-\mu}\left[\alpha_{j'm'}(\nu')\alpha_{jm}(\nu)\right]_{\lambda\mu}\varphi^{\lambda i}_{j(\nu)j'(\nu')}\right) \tag{4.3}$$

properly generalized to the continuum as in I (4.5). Since, by the assumption (4.2), the quasi-particle creation operators (4.1) for continuum states are identical to particle creation operators, the even system with continuum admixtures is in principle treated in the same way as in the case without pairing, considered in I.

The equations to determine the wave function will have the same form as I (4.13) – I (4.17). We shall, however, here introduce the frequently used approximation of separability of the particle-hole forces. This means that in I (4.16), we get

$$\begin{aligned}&\langle\lambda'+|V_\ell|\lambda+\rangle \equiv \langle\mu'\bar{\nu}'|V_\ell|\mu\bar{\nu}\rangle \equiv F_{\mu'\bar{\nu}'}\cdot F_{\mu\bar{\nu}}\\ &\langle\lambda'+|V_\ell|\lambda-\rangle \equiv F_{\mu'\bar{\nu}'}\cdot F^*_{\mu\bar{\nu}}\\ &\langle\lambda+|V_\ell|i\lambda+\rangle \equiv F_{\mu\bar{\nu}}\cdot F^*_{i\bar{\lambda}}\\ &\langle\lambda+|V_\ell|i\lambda-\rangle \equiv F_{\mu\bar{\nu}}\cdot F^*_{i\bar{\lambda}}\ ,\end{aligned} \tag{4.4}$$

etc. Further, since we want in (4.3) to express the collective bosons by the quasi-particle operators, the matrix elements in the RPA equations must be replaced by

$$\begin{aligned}&\langle j_{\mu'}j_{\bar{\nu}'}|\hat{V}_\ell|j_\mu j_{\bar{\nu}}\rangle =\\ &\langle j_{\mu'}j_{\bar{\nu}'}|V_\ell|j_\mu j_{\bar{\nu}}\rangle\, u^{(+)}_{j_{\mu'}j_{\bar{\nu}'}}\, u^{(+)}_{j_\mu j_{\bar{\nu}}}\\ &u^{(+)}_{j_1j_2}\equiv u_{j_1}v_{j_2}+u_{j_2}v_{j_1}\end{aligned} \tag{4.5}$$

and the energies ε_j by the quasi-particle energies

$$E_{j(\nu)}=\sqrt{\left(\varepsilon_{j(\nu)}-\varepsilon_F\right)^2+\Delta^2_{j(\nu)}}\ . \tag{4.6}$$

$$(\Delta_{j(\nu)}=0 \text{ for } \varepsilon_{j(\nu)}>0)$$

The wave functions of the odd system are now (written for discrete components) given as

$$\begin{aligned}|\Psi\rangle_{IM} = &\sum_\nu\Big(a_{0\nu\varsigma}\,\alpha^+_{jm}(\nu)+\sum_{\lambda i j\nu}\left[\alpha^+_{jm}(\nu)Q^{+i}_{\lambda M}\right]_{IM}a^{\lambda}_{j\nu\varsigma}+\\ &+\sum_{\substack{\lambda_1 i_1\lambda_2 i_2\\ jI}}\left[\alpha^+_{jm}(\nu)\left[Q^{+i_1}_{\lambda_1M_1}\cdot Q^{+i_2}_{\lambda_2M_2}\right]_{IM'}\right]_{IM}a^{\lambda_1 i_1\lambda_2 i_2}_{jI\nu\varsigma}\Big)|\Psi_0\rangle\ ,\end{aligned} \tag{4.7}$$

where the Q^{+}'s are the phonon creation operators, defined above, with $\{\psi, \varphi\}$ corresponding to $\{X, Y\}$ and $\{X, Y\}$ of I (4.5), normalized by

$$\sum_{qq'} \left(\psi^{i}_{qq'} \psi^{i'}_{qq'} - \varphi^{i}_{qq'} \varphi^{i'}_{qq'} \right) = \delta_{ii'} . \tag{4.8}$$

Here, the coefficients could be determined by the equation corresponding to I (4.17). Since $\psi^{i}_{qq'}$ and $\varphi^{i}_{qq'}$ will be proportional to $U^{(+)}_{qq'}$, as is seen from (4.2), (4.5), only one particle may be in the continuum.

We can, however, in a realistic situation have one incoming particle, only.

If (4.17) really represented a complete antisymmetric solution with a Hamiltonian, which was symmetric in all particles outside a closed shell, it would be irrelevant whether this incoming particle was represented by the odd particle creation operator or by a term in the two-quasiparticle operators.

We shall in the following assume that incoming particles are only represented by a^{+}; however, we shall follow earlier treatments [7] in assuming that the presence of the odd particle (as well as the phonon-phonon coupling) does not influecne the structure of the phonon states. This means that the phonons can in the continuum at most have an outgoing particle, and that they must therefore be found by solving an eigenvalue problem, which is the one which corresponds to the eigenvalue equation of the last chapter (3.2), with the proper changes (U, V factors and quasiparticle energies instead of ε_ν)

$$Det(\underline{M}) = 0 \tag{4.9}$$

$$\begin{aligned} \langle \xi | M | \eta \rangle = {} & \langle \xi | \tilde{V}_1 | \eta \rangle - \\ & - (t E - E_\lambda) \delta_{\xi\eta} \delta_{\xi\lambda} - \\ & - 2 k_\tau (k_\lambda - s_i k_\tau) \delta_{\xi\eta} \delta_{\xi,\lambda i} , \end{aligned} \tag{4.10}$$

where $t = +$ and $t = -$ correspond to the ψ and φ part of the eigenvectors, respectively, and $\langle \eta | \tilde{V} | \xi \rangle$ is short for the matrix elements of (4.5), whereas

$$E_\lambda = E_{JN} = E_j(\nu) + E_{j'}(\nu') , \quad K_\lambda^{+} = (E - E_j(\lambda))^{1/2} .$$

The equations for the odd system are now reduced to the same type as those met in the continuum shell model, treated in I, chapter 3, with the proper changes, i.e., that the states $|\lambda\rangle = |\mu_\lambda \bar{\nu}_\lambda\rangle$, etc., I (3.3), are replaced by the components of (4.7)

$$\begin{aligned} & |\lambda\rangle_{JM} = \alpha^{+}_{JM}(\nu) |\tilde{0}\rangle , \quad |\lambda\rangle_{JM} = [\alpha^{+}_{j} \alpha^{+}_{j'}]_{JM} |0\rangle \\ & |k, \lambda = 0\rangle_{JM} = \alpha^{+}_{JM} |0\rangle \\ & |k, \lambda \neq 0\rangle_{JM} = [\alpha^{+}_{j} Q^{+}_{j'}]_{JM} |0\rangle , \quad \text{etc.} \end{aligned} \tag{4.11}$$

The introduction of the corresponding pole states, $|i\,\lambda\rangle$ is straightforward following the methods of I, chapter 4.

The interaction, V_1 of I (3.1) is replaced by the quasiparticle-phonon interaction, H_{qp4} which, e.g., can be taken [7] as

$$\begin{aligned} & -\frac{1}{2\sqrt{2}} \sum_{\lambda\mu i} \left(Q^{+i}_{\lambda\mu} + (-)^{\lambda-\mu} Q^{\tau}_{\lambda-\mu} \right) \times \\ & \times \sum_{j_1 j_2 \tau} f^{\lambda}_{j_1 j_2} \frac{V^{(-)}_{j_1 j_2}}{\sqrt{y^{\lambda i}_{\tau}}} \left[\alpha^{+}_{j_1 m_1} \alpha^{-}_{j_2 -m_2} \right]_{\lambda-\mu} + h.c. \\ & \tau = (n, p) \\ & V^{(-)}_{j_1 j_2} = u_{j_1} u_{j_2} - v_{j_1} v_{j_2} . \end{aligned} \tag{4.12}$$

Here $f^{\lambda}_{j_1 j_2}$ is the reduced single-particle matrix element of the multipole operators $\tau^{\lambda} Y_{\lambda\mu}$; the normalization $y^{\lambda i}_{\tau}$ is given in Ref. 7 .

For many applications the continuum admixtures in the phonon may be neglected, and their energies found as real numbers in the usual random phase approximation. In the general case, however, we see that the introduction of decaying (damped) phonons, as above , means that the corresponding energies, e_λ of the equation corresponding to I (3.4) are complex.

Even when all continuum admixtures are neglected, the calculations leading to a wave function of the type (4.7) are often replaced by looking for the so-called strength function, i.e., for the admixtures of a certain component in the solutions. Further, the

exaot strength function is often replaced by an average strength function, whioh gives the averaged oontent of a component in eigenfunctions in an energy interval.

Since the eigenenergies will often lie very dense, the strength function will often correspond to the physioal measurements. An extension of this method to the oase, when oontinuum admixtures are taken into aocount is straightforward. In some cases this will even lead to somewhat simpler caloulations, as we shall see in the following.

Let us suppose that the component in whioh we are interested is the one, which in our model is described by a single particle creation operator, acting on the even vacuum (the first component in (4.7)). This oorresponds, e.g.,to a stripping experiment with the even vacuum as target state.

If this component belongs to the discrete part of the wave function, as will be the oase,if the total energy is smaller than the lowest partiole emission threshold, the calculation of the strength function must follow the usual soheme. This means that the square of the coefficients, which would in principle result from a matrix diagonalization, must be averaged with someweight function, say,

$$|a(z)|^2 = \sum_\tau \varrho(z - E_\tau)\, a_{0\tau}^2 , \qquad (4.13)$$

where τ denotes a solution of the eigenvalue problem of the odd system, E_τ the oorresponding eigenvalue. Here, ϱ is conventionly chosen in the Lorentz form,

$$\varrho(x) = \frac{1}{2\pi}\,\frac{\Delta}{x^2 + \Delta^2/4} . \qquad (4.14)$$

The sum in (4.13) can be turned into an integral of an expression, which has poles at the eigenvalues E_τ . The resolvent

$$R = (z - H)^{-1} \qquad (4.15)$$

has this property and in some simple examples (see,e.g.,8), even the residues will be given directly by the resolvent. It is a necessary condition for this type of calculation to be feasible, that the $|a_\tau|^2$ are given, for real E_τ , in a way which can be analytioally oontinued in some region of the E plane.

Now, also $\varrho(z-z')$ has poles at $z' = z \pm i\frac{\Delta}{2}$ and the average is, by oontour integration, obtained from the residues in these points. The character of this calculation is not changed, even if some of the poles are oomplex.

If the average distanoe between eigenvalues of the system with quasi-particle-phonon ooupling is much smaller than between the quasi-partiole energies in the absenoe of coupling, and if Δ is between these, the result of the averaging oan be expressed by saying that the (analytic) expression for $|a|^2$ has poles, whose real part is near to the quasipartiole energies and with an imaginary part, $\frac{1}{2}\Gamma$ which is proportional to the average of the square of the ooupling /7,8/ .

Some,e.g., stripping oross section will contain a Lorentz faotor

$$f \sim \frac{\Gamma}{(E - E_{p(\tau)})^2 + \frac{1}{4}(\Gamma/2)^2} \qquad (4.16)$$

$$E_{p(\tau)} \sim E_\nu \quad (\text{quasip})$$

$$\Gamma \sim 2\pi \langle \tilde{V}_1^2 \rangle \quad (\times \text{ density of levels in coupling}) . \qquad (4.17)$$

Stripping, leading to a suffioiently narrow single particle resonance state, distributed over a number of oomplex states, may in prinoiple be described in the same way as above. The resonanoe funotions were succossfully used in the desoription of stripping in the simple case where the coupling to other states can be neglected /9/ .

It ought to be mentioned that around threshold for partiole emission, the analytio energy dependence of the amplitudes, needed in the procedure desoribed above, is not fulfilled. This leads to practioal difficulties only for the case of neutrons in S-states, and only in the neighbourhood of the threshold.

If the single particle resonanoe is, as will often be the oase, sufficiently wide, no further averaging is needed in the caloulation of the strength funotion. The same is seen in the elastio scattering. Here, the formalism of I, chapter 3 is again applicable. We shall again assume that the even oore system is desoribed in terms of eigenstates in the RPA-meaning, but with energies whioh oan be complex. Let the only component which can have incoming particles be the one which oorresponds to the ground state of the even system. Now, in the wave funotion (4.7) the summations over ν are in the oontinuum replaced by integrals over K , so we get a set of components

$$\Psi_p\rangle = \int dK\; (a_{0\beta}(K)\, \mathcal{L}^+_{\beta N}(K) +$$

$$+\sum_{\lambda i j} \alpha^{\lambda i}_{\beta\xi}(x)\left[\alpha^{+}_{\beta m}(x)\, Q^{i+}_{\lambda\mu}\right]_{JM} + \tag{4.18}$$

$$+\sum_{\lambda_1\lambda_2 l_1 l_2}{}' \left[\alpha^{+}_{\beta m}(x)\left[Y^{+l_1}_{\lambda_1\mu_1} Q^{+l_2}_{\lambda_2\mu_2}\right]_{IM'}\right]_{JM} \alpha^{\lambda_1\lambda_2 l_1 l_2}_{\beta I J\xi}(x)\Big) \quad \gamma_0 > ,$$

where

$$a_{\xi\xi}(x) = A_\xi\,\delta(x-K_\xi) + b_\xi(x). \tag{4.19}$$

We may as before write

$$b_\xi(x') = (K_\xi^2 - x'^2)^{-1} \sum_i f_{i\xi}(K)\beta_{i\xi'} , \tag{4.20}$$

(ξ channel index)

where

$$f_i^{*}(x) = \frac{\varphi_i(R)\,K}{h_e^{+}(xR)\,2K_i\,(x-K_i)} . \tag{4.21}$$

In solving the equations for the b's or, equivalently, the β's we are led to equations which are formally identical to I (3.8), I(3.9). We may now, as in I, use the G^{+} definition of the singular integrals. In this way, we would come direotly to the T matrix of the scattering. This is in many ways the simplest method. However, it may also have some advantages to use real quantities. This means that the singular integrals must be interpreted in terms of principal values. This method leads, as pointed out by Bloch instead of the T matrix, to the analogous K-matrix. Since this approach is frequently used, we shall stick to that, the changes needed to replace it by the T matrix approach being simple. Note, that we are in our notation following Bloch. The matrix, here called K , is related to the usual K-matrix, see (4.30), (4.31) below.

The main point is that when the principal value definition of the singular integrals is introduced, I (3.11) is replaced by

$$F^{P}_{\lambda i} = \frac{S_i\,\varphi_i^{*}(R)}{K_\lambda^2 - K_i^2} . \tag{4.22}$$

This means that the PP-elements in the M-matrix of I (3.21) are replaced by

$$\langle\lambda' i'|M|i\lambda\rangle = \langle\lambda' i'|V_L|i\lambda\rangle - S_i\,(K_\lambda^2 - K_i^2)\,\delta_{ii'}\,\delta_{\lambda\lambda'}, \tag{4.23}$$

$$\alpha^{P}_{i\lambda} = \beta_{i\lambda}\, S_i \,/\, (K_\lambda^2 - K_i^2) . \tag{4.24}$$

Now, we are interested in elastic scattering, i.e., in the residue β_0 in Blochs notation of the ooefficient $b_0(x)$ at its pole K_λ .

This is just what in I, chapter 3, is called

$$\sum_i \beta_{i0}\, f_{i0}^{*} \quad (=\beta_0). \tag{4.25}$$

It may at this point be advantageous to introduoe a oommon notation for all oomponents, whether they belong to resonanoe poles or not. So for a olass of Λ values

$$|\Lambda\rangle \equiv |i\lambda\rangle \qquad (\lambda > \lambda_B). \tag{4.26}$$

Then, from the last equation of I (3.21), together with I (3.20) we have, with the substitution (4.23)

$$\beta_{\Lambda_0} = S_{\Lambda_0}\,(K_\lambda^2 - K_{\lambda_0}^2)\,\alpha_{\Lambda_0} = \tag{4.27}$$

$$= \sum_\Lambda V_{\Lambda_0\Lambda}\,(\alpha_\Lambda - \tilde{A}_\Lambda),$$

where we have introduced

$$K_\Lambda \equiv K_{\lambda(\Lambda)} \quad , \quad K_\Lambda \equiv K_{i(\Lambda)} \quad , \quad \tilde{A}_\Lambda = f_\Lambda A_\Lambda .$$

Now, eliminating the first right-hand term by means of I (20) we get

$$\beta_{\Lambda_0} = \sum_\Lambda \left(-V_{\Lambda_0\Lambda_0'} + \sum_{\Lambda''\Lambda'} V_{\Lambda_0\Lambda'}\, M^{-1}_{\Lambda'\Lambda''}\, V_{\Lambda''\Lambda_0'}\right)\tilde{A}_{\Lambda_0'} \tag{4.28}$$

(This is, striotly speaking, an elimination only if $V_{\Lambda_0\Lambda_0'} = 0$ which may, however, safely be assumed (see, e.g., ref. 2)). The analogy between (4.28) and Blooh's equations (2.42)–(2.46) should be noted.

The two-step elimination method of Bloch would seem to be the most reasonable thing to use, if the wave funotions at the different steps were very different.

However, our bound state wave functions in chapter I.3 and resonance wave functions as given by I (3.3) have the same struoture. Therefore a one-step elimination, treating oontinuum oouplings on the same footing as those in the discrete part of the wave function, seems reasinable.

A comparison with Bloch's equations (2.47), (2.58) now shows, that if we write (4.28) as

$$\beta_{\lambda_0} = \underline{\underline{K}}\, \underline{\tilde{A}}\,|_{\lambda_0} \tag{4.29}$$

(where equations for other components could have been obtained analogously, and the restriction to $\tilde{A}_\lambda \sim \delta_{\lambda_0}$ is not necessary) then the scattering matrix is obtained as

$$\underline{\underline{S}} = e^{i\delta}\, \underline{\underline{\tilde{S}}}\, e^{-i\delta}, \tag{4.30}$$

$$\underline{\underline{\tilde{S}}} = \frac{1 + i\underline{\underline{K}}}{1 - i\underline{\underline{K}}} . \tag{4.31}$$

Still (4.28) contains terms, corresponding to all couplings, caused by the residual interactions, including the usually neglected ones.

The qualitative picture, which results from (4.28) can again conveniently be obtained by looking at the averaging of the cross section. This can be done by contour integration or in other words by introducing an imaginary part in the energy $(i\Delta_E)$ or momentum $(i\Delta_K)$ equal to the corresponding experimental width. For the average cross section, we have

$$\langle \sigma(E) \rangle_\Delta \approx 2\,(1 - Re\,\langle S(E) \rangle_\Delta)$$

where the contribution to $\langle S \rangle_\Delta$ from β_{λ_0} is obtained from

$$\underline{\alpha}_\Delta = \left(\underline{\underline{M}}\,(K + i\Delta_K)\right)^{-1} \underline{V}\, \underline{\tilde{A}} .$$

Note, however, that when the momentum is in the neighborhood of a single particle resonance K_i, which is wider than Δ_K the imaginary part of the diagonal elements will be dominated by this $Im(K_i)$ and Δ_K may be neglected. The cross sections, corresponding to this single particle resonance must of course again be obtained by an energy (momentum) integration over an interval, corresponding to the width [8] (or a little larger), so $Im(K_i)$ will in this case completely replace $\sum \Delta_K$, the experimental momentum width.

Conclusion

We have here in some details looked at the possibilities of using the pole expansion method of I in nuclear physics problems, particularly concerning the construction of complex, decaying states and strength functions.

In the usual calculation, a number of further simplifying assumptions are introduced, in order to accommodate the diagonalization of inversion of what corresponds to our matrix $\underline{\underline{M}}$.

Similar assumption can immediately be introduced in the resonance function method. What we have in mind is, e.g., the assumption of constant matrix elements in RPA or pairing calculations, or similar simplifications in the particle-phonon matrix elements. It should still be kept in mind, however, that when the basis is extended, the effective interactions used in a truncated basis must be changed, in order to obtain realistic results.

Here, again the general principle of using interactions, which reproduces the energy spectra or parts of them as well as possible, may be followed, then looking for the possible improvement in other measurable quantities with the extension of the basis. The most nearlying quantity is here the particle decay width as is seen in elastic scattering or (δ, n) and (γ, p) processes. This is immediately obtained from the calculations, sketched above, which obviously take into account, in the terminology of, e.g., ref. [5] both $\Gamma^\downarrow$ and $\Gamma^\uparrow$.

Concrete numerical calculations are under preparation; they will be published elsewhere.

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Банг Е., Гареев Ф.А., Ершов С.Н. Резонансные состояния в структурных вычислениях (продолжение) E4-81-415

Обсуждается возможность использования метода разложения по полюсным функциям /согласно теореме Миттаг-Лефиера/ для описания ядерных состояний, лежащих в непрерывном спектре, рассматриваются некоторые математические свойства разложений по резонансным функциям, приводятся формулы для вычисления одночастичных силовых функций. Особое внимание уделяется описанию сложных, распадающихся состояний, компоненты которых содержат не более одной частицы в континууме. Развитый метод очень прост в практических расчетах, так как в результате получается система алгебраических уравнений, по форме почти совпадающих с уравнениями оболочечной модели.

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Bang J.M., Gareev F.A., Ershov S.N. Resonant States in Structure Calculations (Continued) E4-81-415

Some applications of the expansion method for description of continuum nuclear states are discussed. Some mathematical properties of resonance expansion are considered. Formulae are given for calculation of one particle strength function. Description of the complex decaying states containing only components with one particle in the continuum are given. The method is very simple since it leads to a system of algebraic equations.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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