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RESONANT STATES  
IN STRUCTURE CALCULATIONS

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Резонансные состояния в структурных вычислениях

Строго математически рассмотрено полюсное разложение (по теореме Миттаг-Леффлера в формулировке Коши) волновых функций, амплитуд рассеяния и функций Грина при положительных энергиях. Получен и обсуждается общий вид этих разложений для потенциалов конечного радиуса взаимодействия, а также для кулоновского потенциала взаимодействия. Полученные ряды сходятся равномерно на всей комплексной плоскости  $k$  за исключением полюсов. Обсуждается ряд примеров применения метода в структурных вычислениях с включением состояний непрерывного спектра, в частности, оболочечная модель и метод случайной фазы. Предложенный метод очень прост в практических расчетах, так как в результате получается система алгебраических уравнений, по форме почти совпадающих с уравнениями оболочечной модели.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1978

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Resonant States in Structure Calculations

The expansion in resonant states is suggested as a method for extension of nuclear structure calculations by including continuum states. The method is shown to lead to considerable simplifications, as compared to previous methods, in the calculation of one-particle-one-hole excitations, including giant multipole resonances, and ground state correlations.

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

Communication of the Joint Institute for Nuclear Research. Dubna 1978

## 1. INTRODUCTION

The problem of nuclear structure calculations, with inclusion of continuum states has recently called for a considerable attention.

One may here distinguish between at least two problems. The first, which is mainly a mathematical one, concerns the fact that the bound single particle states of the nuclear potential do not form a complete set. Therefore a diagonalization of the full Hamiltonian, including residual interactions, will involve continuum states as well. The presence of such continuum admixtures in bound states is in general not very important for calculation of energies for the ground states, but it can be of considerable significance for cross sections of nuclear reactions<sup>1/</sup>. The way in which such admixtures should be taken into account must therefore depend on which type of reaction amplitudes one wants to calculate. For direct transfer processes, e.g., the complete set of Sturm-Liouville functions was successfully applied as expansion basis.

The continuum admixtures come into play in a more direct physical way, however, when we look at such reactions as  $(\gamma, p)$ ,  $(p, \gamma)$ ,  $(\gamma, n)$ , etc., and at electromagnetic transitions to states above the particle emission threshold in general. The giant electromagnetic multipole resonances lie in this region, and since they can be studied by means of the processes just mentioned, some inclusion of unbound states in the description of these excitations is unavoidable. It is further clear from the very nature of the giant resonances that their

wave functions must be obtained by some configuration mixing calculation, using the residual interactions, predominantly of the particle-hole type.

Such calculations, with inclusion of continuum admixtures, are in general complicated, compared, e.g., to the model problems treated in ref.<sup>1,2/</sup> by the presence of many channels, even if we restrict ourselves to those with only one-particle in the continuum.

A very consistent way of solving such problems is the method of coupled channels<sup>3,4,5/</sup>. Here, the continuum states are found as solutions of a system of coupled equations, which are in principle of integro-differential type. The great complexity of these equations has, however, restricted the application of this method to light nuclei, and the residual forces, responsible for the channel coupling, to  $\delta$ -forces.

When an expansion in a discrete set of basis states is used, the last restrictions can be removed, and the first one is also becoming less serious. However, the methods for discretization, which have been suggested<sup>6,7/</sup>, based either on replacing the energy-continuum by a more or less arbitrary discrete set of energies, or on expansion of the continuum functions or a fixed basis, say, of harmonic oscillator functions, are still extremely complicated.

We shall therefore here try to solve the problem along the same lines as in ref.<sup>1/</sup>. The main point is here that, although the non-orthogonality of the resonance states presents difficulties for a straight-forward diagonalization of the Hamiltonian with these states as basis, the Mittag-Leffler expansion of the Green function leads to a determination of the relevant expansion coefficients in terms of matrix elements of the residual interactions between resonant states. We are here using the fact that the scattering states appear only in the calculation of matrix elements, with operators which go rapidly to zero with increasing distance from the center of the nucleus, so that we only have to integrate up to a finite distance  $r=R$ . In this respect, our method is similar to that of Birkholz<sup>7/</sup>.

Although it could be of interest to treat the entire problem by Green function technique<sup>8/</sup>, we shall here, for the sake of simplicity, treat the bound and unbound states in different ways, like in refs.<sup>1-7/</sup>.

## 2. THE MITTAG-LEFFLER EXPANSIONS OF GREEN'S FUNCTION AND OF THE SCATTERING STATES

Since the Mittag-Leffler expansions of Green's function and of the scattering states were discussed in detail in previous work, we shall here just, without proof, recapitulate the properties of these expansions.

With certain restrictions on the potential, e.g., that it is zero outside a radius  $R$ , the radial part of single particle Green's function has the Mittag-Leffler expansion

$$G_{\rho}(k; r, r') = \sum_i \frac{\phi_i(r)\phi_i(r')}{2k_i(k-k_i)} \quad r, r' < R \quad (2.1)$$

Here the  $k_i$  are ( $G^{\pm}$ - are obtained as the limits  $G(\pm|k|+iy)_{y \rightarrow 0}$ ) all poles of the  $S$ -matrix,  $\phi_i$  are the corresponding residual functions, satisfying  $(\frac{d}{dr} + 1)$

$$\left(-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + V(r) - k_i^2\right)\phi_i(r) = 0. \quad (2.2)$$

The  $\phi$ 's are non-orthogonal, their normalization is given in ref.<sup>1/</sup>, we quote the relation for  $\ell=0$

$$\int_0^R dr \phi_n(r)\phi_m(r) + i \frac{\phi_n(R)\phi_m(R)}{k_n+k_m} = \delta_{nm} \quad (2.3)$$

For the bound state poles, the normalization is identical to the usual one. As shown in<sup>1/</sup>, Green's function in the space of continuum states, PGP in Feshbach notation, can be written

$$G_p = \sum_i \frac{\phi_i(r)\phi_i(r')}{2k_i(k-sk_i)} \quad (2.4)$$

Here  $s = -1$  for bound state poles,  $s = +1$  for antibound, resonant and mirror-resonant poles. Note the occurrence of bound states in  $G$ ; a relation like (2.3) will *not* allow us to construct a projection operator  $|\phi_i\rangle\langle\phi_i|$ .

In order to avoid confusion, we shall stick to the notation that the bound state indices, as well as other discrete quantum numbers, which correspond to orthogonality relations are denoted with Greek letters, whereas continuous variables, *and the pole* indices, are denoted with Latin letters. This means that in our expressions the same function may occur both as  $\phi_n$  and as  $\phi_\nu$ , according to whether it appears in the expansion of  $G_p$  or of  $Q\Psi$  (the bound state part of the wave function).

The scattering states  $\Psi_\ell^+(k,r)$  satisfy, for  $r < R$ , the same Schrödinger equation as  $G_\ell(k,r,R)$ , therefore it is proportional to this and has the same type of Mittag-Leffler expansion

$$\Psi_\ell^+(k,r) = \sum_i f_i(k)\phi_i(r); \quad r \leq R$$

$$f_i(k) = \frac{c_i(k)}{k-k_i} = \frac{\phi_i(R) \cdot k}{2k_i(k-k_i)h_\ell^+(kR)} \quad (2.5)$$

For  $r > R$ , (2.5) will in general not converge, but  $\Psi_\ell^+$  is nevertheless easily calculable, knowing the poles of  $S$ . As mentioned above, we are, however, only interested in matrix elements with  $\Psi^+$  which are well approximated by integrating over  $r$  from 0 to  $R$ .

### 3. CONTINUUM SHELL MODEL CALCULATION

We shall here follow the usual scheme of continuum shell model calculations<sup>9,10</sup>. We shall consider a Hamiltonian of a system of  $A$  nucleons

$$H = H_1 + T + V + V_1 = H_0 + V_1, \quad (3.1)$$

where  $H_1$  is the Hamiltonian of the  $(A-1)$  nucleon system;  $T+V$ , the kinetic energy and shell-model potential ("optical potential", but "real") of one extra nucleon; and  $V_1$ , a residual interaction.

The total wave function is now expanded in terms of discrete and continuous eigenfunctions of  $H_0$

$$\Psi = Q\Psi + P\Psi =$$

$$= \sum_\Lambda a_\Lambda |\Lambda\rangle + \sum_\lambda \int dk a_\lambda(k) |k\lambda\rangle. \quad (3.2)$$

As an example, we may think of particle-hole states (bar means hole)

$$|\Lambda\rangle = |\mu_\Lambda\rangle |\bar{\pi}_\Lambda\rangle$$

$$|k\lambda\rangle = \Psi_\lambda^+(k,r)|\lambda\rangle$$

$$= \Psi_\lambda^+(k,r) Y_{\ell_\lambda m_\lambda} > \bar{\pi}_\lambda >. \quad (3.3)$$

We shall here, for simplicity, omit explicit antisymmetrization, which essentially just means the inclusion of exchange terms in the matrix elements of  $V_1$ .

If we write

$$a_\lambda(k) = A_\lambda \delta(k-k_\lambda) + \frac{2}{\pi} b_\lambda(k)$$

$$k_\lambda^2 = E - e_\lambda \quad (3.4)$$

(in the example  $e_\lambda = |e_{\pi\lambda}|$ ), we see that  $A_\lambda$  describes the boundary conditions of  $\Psi$ . Note that  $k_\lambda$ , defined by (3.4), should not be confused with the poles,  $k_i$ . Now  $b_\lambda$  is determined, together with  $a_\Lambda$ , by the system

of integral equations obtained by inserting (3.2) in the Schrödinger equation and multiply by  $\langle \Lambda' |$  and  $\langle k' \lambda' |$

$$\sum_{\Lambda} \langle \Lambda' | E_{\Lambda'} - E + V_1 | \Lambda \rangle a_{\Lambda} + \frac{2}{\pi} \sum_{\lambda} \int_0^{\infty} dk \langle \Lambda' | V_1 | k \lambda \rangle b_{\lambda}(k) \quad (3.5)$$

$$= - \sum_{\lambda} \langle \Lambda | V_1 | k_{\lambda} \lambda \rangle A_{\lambda}$$

$$\begin{aligned} (k'^2 - k_{\lambda'}^2) b_{\lambda'}(k') + \sum_{\Lambda} \langle k' \lambda' | V_1 | \Lambda \rangle a_{\Lambda} \\ + \frac{2}{\pi} \sum_{\lambda} \int_0^{\infty} dk \langle k' \lambda' | V_1 | k \lambda \rangle b_{\lambda}(k) = - \sum_{\lambda} \langle k' \lambda' | V_1 | k_{\lambda} \lambda \rangle A_{\lambda} \end{aligned} \quad (3.6)$$

Since the matrix elements here contain a short range force  $V_1$  and hole states with a rapid fall off the wave function with increasing distance from the center of the nucleus, the integral may be cut off at  $r_1 = R_1$ ,  $r_2 = R$  without changing their values if  $R$  is sufficiently large.

If we now introduce the Mittag-Leffler expansion (2.5) of  $\Psi_{\lambda}^{+}(k, r)$  in the  $\langle k' \lambda' |$ , we see that from (3.6) we obtain

$$b_{\lambda'}(k') = (k_{\lambda'}^2 - k'^2)^{-1} \sum_i f_{i(\lambda')}^{*} (k') \beta_{i\lambda'} \quad (3.7)$$

where the  $\beta_{i\lambda'}$  are to be determined below.

So the integrand in (3.5) and (3.6) is singular. Nevertheless, we do not need, at this point, to specify in what way we shall treat this singularity. This is only a matter of the choice of  $A_{\lambda}$ .

So, from (3.5), (3.6) we get, using again the expansion (2.5) for the bra  $\langle k' \lambda' |$  and for the ket  $| k_{\lambda} \lambda \rangle$

$$\begin{aligned} (E_{\Lambda'} - E) a_{\Lambda'} + \sum_{\Lambda} \langle \Lambda' | V_1 | \Lambda \rangle a_{\Lambda} \\ + \sum_{\lambda} \frac{2}{\pi} \int_0^{\infty} dk \langle \Lambda' | V_1 | \Psi_{\lambda}^{+}(k, r) \lambda \rangle = \frac{1}{k_{\lambda}^2 - k'^2} \sum_i f_{i\lambda}^{*} (k) \beta_{i\lambda} \\ = - \sum_{i\lambda} \langle \Lambda' | V_1 | \phi_{i\lambda} \rangle f_{i\lambda}(k_{\lambda}) A_{\lambda} \end{aligned} \quad (3.8)$$

$$\begin{aligned} \sum_{\Lambda} \langle \lambda' \phi_{i\lambda'} | V_1 | \Lambda \rangle a_{\Lambda} - \beta_{i\lambda'} \\ + \sum_{\lambda_i} \frac{2}{\pi} \int_0^{\infty} dk \langle \phi_{i\lambda'} | V_1 | \Psi_{\lambda}^{+}(k, r) \lambda \rangle = \frac{1}{k_{\lambda}^2 - k'^2} f_{i\lambda}^{*} \beta_{i\lambda} \\ = - \sum_{i\lambda} \langle \lambda' \phi_{i\lambda'} | V_1 | \phi_{i\lambda} \rangle f_{i\lambda}(k_{\lambda}) A_{\lambda} \end{aligned} \quad (3.9)$$

In obtaining (3.9) we have used the uniqueness of the Mittag-Leffler expansion of  $\langle k' \lambda' |$  to equate the pole terms with  $i'$  on both sides. So, the problem of constructing  $\Psi >$  is reduced to finding the  $a, \beta$  from (3.8), (3.9), with the  $A$ 's given. In matrix notation, we may write (3.8), (3.9),

$$\underline{\underline{W}} \begin{pmatrix} a \\ \beta \end{pmatrix} = \underline{\underline{V}}_1(\underline{\underline{f}}A) \quad (3.10)$$

$$\begin{pmatrix} a \\ \beta \end{pmatrix} = \underline{\underline{W}}^{-1} \underline{\underline{V}}_1(\underline{\underline{f}}A), \quad (3.11)$$

We see that the matrix  $\underline{\underline{V}}_1$  and the vector  $(\underline{\underline{f}}A)$  are obtained in a simple form from the Mittag-Leffler expansion; particularly the energy dependence of  $(\underline{\underline{f}}A)$ , through  $k_{\lambda}$  in  $(k_{\lambda} - k_j)^{-1}$ , is easily taken into account. The greatest advantage of the present method lies, however, in the calculation of the matrix  $\underline{\underline{W}}$ .

Here we have matrix elements, which in the particle-hole case can be written

$$\langle \Lambda' | W | \lambda i \rangle = \langle \Lambda(r_1, r_2) | V_1(r_1, r_2) | F_{\lambda i}(r_1), \bar{\pi}_{\lambda}(r_2) \rangle \quad (3.12)$$

$$\langle \lambda' i' | W | \lambda i \rangle = \langle \lambda' i'(r_1, r_2) | V_1(r_1, r_2) | F_{\lambda i}(r_1), \bar{\pi}_{\lambda}(r_2) \rangle - \delta_{\lambda\lambda'} \delta_{ii'} \quad (3.13)$$

where

$$F_{\lambda i}(r) = \int_0^{\infty} dk \Psi_{\lambda}^+(kr) (k_{\lambda}^2 - k^2)^{-1} f_{i\lambda}^*(k) \quad (3.14)$$

Now

$$G_{\lambda, p}^{(\pm)}(k_{\lambda}; r, r') = \frac{2}{\pi} \int_0^{\infty} dk \Psi_{\lambda}^+(kr) (k_{\lambda}^2 - k^2)^{-1} \Psi_{\lambda}^{+*}(kr') \quad (3.15)$$

$$k^{\pm} = \begin{cases} \pm |k| + i|\eta| & k^2 > 0 \\ \eta & \eta \rightarrow 0 \\ i|k| & k^2 < 0 \end{cases}$$

So, if we interpret the integrals in (3.14) and (3.15) in the same way, we can write

$$G_{\lambda, p}^{(\pm)}(k_{\lambda}; r, r') = \sum_i F_{\lambda i}^{(\pm)}(r) \phi_i^*(r') \quad (3.16)$$

Comparing this with (2.4), and using once more the uniqueness of the pole expansion, we get

$$F_{\lambda i}^{(\pm)}(r) = \frac{\phi_i^*(r)}{2k_{\tilde{i}}(k_{\lambda}^{\pm} - sk_{\tilde{i}})} \quad (3.17)$$

where  $k_{\tilde{i}}$  is the mirror pole of  $k_i$ :

$$\text{Re}(k_{\tilde{i}}) = -\text{Re}(k_i); \quad \text{Im}(k_{\tilde{i}}) = \text{Im}(k_i); \quad \phi_{\tilde{i}} = \phi_i^*$$

So we see, that the whole calculation is reduced to calculation of matrix elements of one type, e.g.,

$$\langle \lambda' i' | V_1 | i \lambda \rangle = \langle \lambda' \bar{\pi}_{\lambda}(r_2) | \phi_{i\lambda}(r_1) | \lambda \rangle \quad (3.18)$$

$$V(r_1, r_2) | \phi_{i\lambda}(r_1) \bar{\pi}_{\lambda}(r_2) \rangle$$

We now introduce the notation

$$\alpha_{i\lambda}^{\pm} = \frac{\beta_{i\lambda}}{2k_{\tilde{i}}(k_{\lambda}^{\pm} - sk_{\tilde{i}})} \quad (3.19)$$

Then (3.11) can be written

$$\underline{a} = \underline{M}^{-1} \underline{V}_1(\underline{fA}) \quad (3.20)$$

with

$$\langle \Lambda' | M | \Lambda \rangle = \langle \Lambda' | V | \Lambda \rangle - (E - E_{\Lambda}) \delta_{\Lambda' \Lambda}$$

$$\langle \lambda' i' | M | \lambda \rangle = \langle \lambda' \bar{\pi}_{\lambda} | \phi_{i\lambda} | V_1 | \lambda \rangle$$

$$\langle \Lambda' | M | i \lambda \rangle = \langle \Lambda' | V_1 | \phi_{i\lambda}^* \bar{\pi}_{\lambda} \rangle$$

$$\langle \lambda' i' | M | i \lambda \rangle = \langle \lambda' \bar{\pi}_{\lambda} | \phi_{i\lambda} | V_1 | \phi_{i\lambda}^* \bar{\pi}_{\lambda} \rangle$$

$$- 2k_{\tilde{i}}(k_{\lambda} - sk_{\tilde{i}}) \delta_{ii'} \delta_{\lambda\lambda'} \quad (3.21)$$

We see that M has the simple form of a symmetric, complex matrix, where only the diagonal elements are energy-dependent. Note that the diagonal matrix elements contain the square of the  $\phi_{\tilde{i}}$ 's, not the absolute square, as also was the case of the normalization integral, etc.

We see that the four terms in (3.21) correspond to what in the continuum shell model is called  $H_{QQ}$ ,  $H_{PQ}$ ,  $H_{QP}$  and  $H_{PP}$  respectively. Any formula, where one or more of these terms is small and can be treated as a per-

turbation, is easily obtained from (3.20), (3.21). When we impose the boundary condition of no in- and outgoing waves in any channel, (3.10) becomes a homogeneous equation, which is solved for eigenvalues of the energy.

#### 4. THE RANDOM PHASE APPROXIMATION

In the preceding chapter, we did not need to specify the states  $|\Psi\rangle$ , but it is obvious, that in heavier nuclei, the problem will become very difficult to handle when states with more than one particle and one hole are included. Also, it should be mentioned, that the way of handling continuum admixtures, presented here and in the references we have quoted, are not easily extended to such states.

A way to overcome this difficulty with the bound states is the Random Phase Approximation. The use of this approximation in problems which involve continuous states was suggested by Krewals et al.<sup>11/</sup> In the preceding chapter, second quantization was not introduced, since the antisymmetrization is trivial, and since we wanted to give the formulas a general shape, fit for any description of the (A-1)-system. We shall in this chapter keep the notation of the preceding one.

Here, however, second quantization is nearly unavoidable, and we shall write

$$H_0 = \sum_{\nu} e_{\nu} a_{\nu}^{\dagger} a_{\nu} + \sum_{\mu} \int_0^{\infty} dk e_{\mu}(k) a_{\mu}^{\dagger}(k) a_{\mu}(k) \quad (4.1)$$

$$-V_1 = \sum_{\nu\lambda\mu i} \int \langle \nu\bar{\lambda} | V | \mu\bar{i} \rangle_{an} a_{\nu}^{\dagger} a_{\lambda} a_{\mu} a_{i}^{\dagger} \quad (4.2)$$

Here  $a_n$  means that the matrix element is antisymmetrized. The integral sign in (4.2) means that for such indices, which correspond to continuum states, the sum is replaced by an integral.

Since our continuum states are orthonormalized by

$$\frac{2}{\pi} \langle \mu | \int_0^{\infty} dr \Psi_{\mu}^{+\dagger}(k, r) \Psi_{\nu}^{+}(k', r) \nu \rangle = \delta_{\mu\nu} \delta(k-k') \quad (4.3)$$

we must also have

$$[a_{\mu}^{\dagger}(k), a_{\nu}(k')] = \delta_{\mu\nu} \delta(k-k'), \quad (4.4)$$

where  $a_{\mu}^{\dagger}(k)$  creates a particle in a state  $\sqrt{\frac{\pi}{2}} \Psi_{\mu}^{+}(kr) |\mu\rangle$ . The idea is now to construct operators

$$\begin{aligned} Q_J^{+}(E) = & \sum_{\mu > \epsilon_F} \sum_{\nu} X_{\mu\nu}(E) (a_{\mu}^{\dagger} a_{\nu})_J - Y_{\mu\nu}(E) (a_{\nu}^{\dagger} a_{\mu})_J \\ & + \sum_{\mu > \epsilon_F} \int dk \{ x_{\mu\nu}(k, E) (a_{\mu}^{\dagger}(k) a_{\nu})_J \\ & - y_{\mu\nu}(k, E) (a_{\nu}^{\dagger} a_{\mu}(k))_J \} \end{aligned} \quad (4.5)$$

such that within the usual approximation of random phases

$$[H, Q_J^{+}(E)] = E Q_J^{+}(E). \quad (4.6)$$

The ground state is the correlated vacuum  $|\tilde{0}\rangle$ , defined by

$$Q_J(E) |\tilde{0}\rangle = 0. \quad (4.7)$$

In this state there will be no free particles. The excited states have the form

$$|\Psi\rangle = \prod_i Q_{J_i}^{+}(E_i) |\tilde{0}\rangle \quad E = \sum_i E_i \quad (4.8)$$

The boundary conditions are so that the state  $Q_J^{+}(E) |\tilde{0}\rangle$  can have one free particle, with ingoing and/or outgoing waves, etc. Inserting (4.5) in (4.6) and equating the coefficients of  $a_{\sigma}^{\dagger} a_{\rho}$  on both sides, we obtain a set of coupled, inhomogeneous equations for the  $X, Y, x$  and  $y$ . Here we may, in the same way as we wrote the expression (3.4), conclude that (with  $\tau = (\mu, \nu)$ ) the boundary conditions are defined by  $A_{\tau}$  in



$$x_r(k) = A_r \delta(k - k_{r+}) + \frac{2}{\pi} b_{r+}(k) \quad (4.9)$$

$$y_r(k) = \frac{2}{\pi} b_{r-}(k), \quad (4.10)$$

where

$$k_{r\pm}^2 = \pm E - |e_{\bar{\nu}}(r)| \quad (4.11)$$

and, just as we derived (3.7), we get

$$b_{r\pm}(k) = (k_{r\pm}^2 - k^2)^{-1} \sum_i f_{i(r)}^*(k) \beta_{ir\pm} \quad (4.12)$$

The two signs in  $k_{r\pm}$ , determined by (4.11), should not be confused with the two signs in  $k_{\lambda}^{\pm}$ , corresponding to  $G^+$  and  $G^-$ . Actually,  $k_{r-}$  is, as is seen from (4.11), always purely imaginary for  $E > 0$ .

In order to get our equations on a similar form as (3.20) we introduce

$$a_{it} = \frac{\beta_{it}}{2k_{\lambda_t}^r - s_i k_{\lambda_t}^-} \quad (4.13)$$

$$t = \pm, r = \pm \quad (\text{and } s = \pm)$$

and

$$\begin{aligned} a_{\Lambda+} &\equiv X_{\mu\nu} \\ a_{\Lambda-} &\equiv Y_{\mu\nu} \quad (\Lambda \equiv (\mu, \nu)). \end{aligned} \quad (4.14)$$

Then, finally, we get

$$\underline{a} = \underline{M}^{-1} \underline{V}_1(\underline{fA}) \quad (4.15)$$

with

$$\begin{aligned} \langle \Lambda' + | V_1 | \Lambda + \rangle &= \langle \mu' \bar{\nu}' | V_1 | \mu \bar{\nu} \rangle \\ \langle \Lambda' + | V_1 | \Lambda - \rangle &= \langle \mu' \bar{\nu}' | V_1 | \bar{\nu} \mu \rangle \end{aligned} \quad (4.16)$$

$$\langle \Lambda + | V_1 | i\lambda + \rangle = \langle \mu \bar{\nu} | V_1 | i\bar{\lambda} \rangle$$

$$\langle \Lambda + | V_1 | i\lambda - \rangle = \langle \mu \bar{\nu} | V_1 | \bar{\lambda} i \rangle,$$

where the exchanged order of the indices just means that we are looking at exchange terms.

$$\langle i\lambda_t^r | fA \rangle = f_{i\lambda} (k_{\lambda_t}^r) A_{\lambda}$$

$$\langle a | M | \beta \rangle = \langle a | V | \beta \rangle - (tE - E_{\lambda}) \delta_{a\beta} \delta_{a, \Lambda_t}$$

$$-2k_{\lambda_t}^r (k_{\lambda_t}^r - s_i k_{\lambda_t}^-) \delta_{a\beta} \delta_{a, \lambda_{i_t}} \quad (4.17)$$

Note that although  $k_{\lambda-}$  lie on the positive imaginary axis, as also the bound state poles, the factor  $(k_{\lambda_t} - s_i k_{\lambda_t}^-)$  never becomes zero, since for those poles  $s_i = -1$ . So no singularity appears in our expression.

## CONCLUSION

We have here presented some methods of including continuum states in nuclear structure calculations. The main purpose of calculating such wave functions must be the description of nuclear excitations with energies above nucleon emission threshold. This is the energy region of the giant resonances, and the wave functions, obtained in the above way, seem to provide the most realistic description of these. In particular, the calculation of cross sections of such processes as  $(\gamma, p)$   $(p, \gamma)$ , etc., must

be sensitive to a realistic description of the continuum-particle-hole wave functions.

In this connection, it should be mentioned, that most of the polarization effects, which are generally introduced in calculations of such cross sections are already included in such wave functions. Therefore the transition amplitudes should be directly calculated from matrix elements of one-particle operators with these states.

Presumably, the first suggested method, which is close to the coupled channels formalism should be preferred in calculations of states in lighter nuclei, whereas the random phase approach would be advantageous for heavier nuclei.

Comparing the expressions (3.20), (3.21) and (4.15) - (4.18) with the corresponding ones of refs.<sup>7</sup> and<sup>11</sup>, we see that a large simplification is obtained by introducing the resonance expansions. In these works the continuum states, are, still for  $r < R$ , expanded in an arbitrary, complete set of functions. Then the Green function must also be calculated in this representation. Here it is non-diagonal, and each matrix element is obtained by a numerical integration over  $k$  of  $(k^2 - k_\lambda^2)^{-1}$  multiplied with two different,  $k$ -dependent coefficients. Still, this integration must be performed for many values of  $k_\lambda$ . In such an approach, the uniqueness of the expansion is granted by the orthogonality of the basis functions (provided  $R$  is sufficiently large). With the present method, it is a consequence of the uniqueness of the Mittag-Leffler expansion.

The convergence of the different approaches is a complicated question, which may possibly only be investigated numerically. In this connection, it should be mentioned that preliminary investigations have shown the convergence of the Mittag-Leffler expansion to be fast, especially in the single particle resonance region. The fact, that not only the real part of  $k_i$  is increasing with  $i$ , but also the imaginary part, improves this convergence in a way which is not obtained for other basis sets.

It should be noted also that since Green's function we use lies strictly in the  $P$ -space no question of non-orthogonality between approximated continuum states

and bound states arise; neither will the fulfillment of the Pauli principle cause any trouble.

The numerical results of Krewald et al.<sup>11</sup> show some peculiar anomalies, particularly as concerns the giant dipole resonance. It is difficult to say, whether this is connected with any of the mentioned calculational problems.

Another problem, which may cause trouble, and where a warning may be appropriate, is the following.

Random phase, as well as most other nuclear structure calculations, are generally made with residual interactions, which are model forces, with coupling constants chosen so as to give reasonable results, *when operating within a given space*. When the space is enlarged, some change of these interactions will in general be appropriate, but as far as the interactions are not obtained from first principles, this is a somewhat ambiguous task. As a general principle one may perhaps suggest that the main feature of the *spectra* should be conserved with such a modification, so that improvements would mainly concern the cross sections of different processes, in our case, e.g.,  $(\gamma, p)$ .

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