Letters to the Editor

ON THE COMPUTATION OF THE ENERGY MATRIX OF A SYSTEM OF IDENTICAL PARTICLES IN A STATE WITH GIVEN SPIN

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IN the papers of the author [1,2] a method was developed for the computation of the matrix elements for a system of identical particles in those cases when all the properties of the system are determined by the coordinate wave function and central symmetry is present. Formulas were obtained expressing the matrix elements for an arbitrary many shell configuration in terms of one- or two-particle matrix elements and fractional parentage coefficients. In the expressions for these coefficients enter the matrix elements of the transformation matrices of the permutation and rotation groups. In this note it is reported that the transformation matrices of the permutation group, needed for the computation of matrix elements of two-shell configurations, have been tabulated for all possible symmetries of systems with a total number of particles from three to six. [3] The second part of the tables contains matrices of the permutation group, which enter into the expressions for the matrix elements of the two-particle interaction operator G for systems in a field of arbitrary symmetry when the angular momentum is not conserved. [1)]

For the case of N particles in a field of arbitrary symmetry one may obtain in the Heitler-London approximation the following formula for the matrix elements of the operator G:

$$\langle [\lambda](t)|G|[\lambda](\bar{t})\rangle = \sum_{i<j}^{N} \sum_{\lambda' r' \lambda''} \langle [\lambda](r'\lambda'')|P_{ij}^{(2)}|[\lambda](t)\rangle \times \langle [\lambda](r'\lambda'')|P_{ij}^{(2)}|[\lambda](\bar{t})\rangle\, g_{ij,ij}^{[\lambda'']} \quad (1)$$

(for notation see [1]). The Yamanouchi symbol t labels states corresponding to permutation symmetry [λ]. The number of physically different states, under the assumption that none of the single-particle functions coincide, is equal to the dimension of the irreducible representation of the permutation group with the symmetry scheme [λ]: [2)]

$$g_{ij,ij}^{[\lambda'']} = \begin{cases} g_{ij,ij} + g_{ij,ji} & [\lambda''] = [2] \\ g_{ij,ij} - g_{ij,ji} & [\lambda''] = [1^2] \end{cases},$$
$$g_{ij,ji} = \langle \varphi_i \varphi_j | G | \varphi_j \varphi_i \rangle. \quad (2)$$

The permutations $P_{ij}^{(2)}$ take the number N-1 into the i-th place and the number N into the j-th place with preservation of the increasing ordering of the numbers and are expressed by cycles as follows:

$$P_{ij}^{(2)} = \begin{cases} P_{NN-2\ldots j-1\, j-2\ldots iN-1\, N-3\ldots j} & \text{N-j odd} \\ P_{NN-2\ldots j} P_{N-1\, N-3\ldots j-1\, j-2\ldots i} & \text{N-j even} \end{cases} \quad (3)$$

Tables of the matrix $P_{ij}^{(2)}$ needed in computations using Eq. (1) have been prepared for systems with particle number N from 3 to 6.

As a result, the usual tedious calculation of matrix elements reduces simply to the sum of two-particle integrals with coefficients taken from the tables. [4] In writing the diagonal matrix element of the operator G each term of the corresponding column of the matrix $P_{ij}^{(2)}$ should be taken squared, and in writing the off-diagonal matrix elements the product of the columns corresponding to the Yamanouchi symbols t and $\bar{t}$ should be taken.

The existence of point symmetry allows one to lower the order of the secular equation. To this end it is necessary to form out of the functions with given permutation symmetry linear combinations that transform according to the irreducible representations Γ of the point group that enter into the decomposition [λ] → Γ. The procedure for finding such linear combinations is given in [5].

[1)] These tables will be sent on request from the L. Ya. Karpov Physico-chemical Institute.

[2)] We note that for quantum chemistry one obtains a simple method for the determination of the number of so-called structures (see [4]).

[1] I. G. Kaplan, JETP **41**, 560 (1961), Soviet Phys. JETP **14**, 401 (1962).

[2] I. G. Kaplan, JETP **41**, 790 (1961), Soviet Phys. JETP **14**, 790 (1962).

[3] I. G. Kaplan, Tablitsy transformatsionnykh matrits gruppy perestanovok, vkhodyashchikh v koordinatnye genealogicheskie koèffitsienty (rotaprint), 1962 (Tables of Transformation Matrices of the Permutation Group, that Enter into the Coordinate Fractional Parentage Coefficients).

[4] H. Eyring, J. Walter, and G. Kimball, Quantum Chemistry, J. Wiley & Sons, 1944 (Russ. Transl. IIL, 1948).

[5] I. G. Kaplan, Trudy II Vsesoyuznogo soveshchaniya po kvantovoi khimii, 1962 (Proceedings of the II All-Union Conference on Quantum Chemistry);

Litovskiĭ fizicheskiĭ sbornik (Lithuanian Physics Collection), in press.

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63

SOME REMARKS ON LOW-ENERGY ππ SCATTERING

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RECENTLY many authors [1-5] solved numerically the equations of low-energy pion scattering. Among the solutions obtained by Serebryakov and Shirkov there are some with resonances in the A_0-wave and in the A_1-wave (waves with I = S = 0 and I = S = 1, respectively).

The resonance in the p-wave is completely due to the large A_0-wave. In the absence of resonance in the A_0-wave, there are no solutions with p-wave satisfying the threshold condition

$$A_1(\nu)|_{\nu=0} = 0.$$

For the width of the p-resonance there is an upper limit of 50 MeV, connected with saturation of the A_0-wave. In many papers [2-5], the Chew-Mandelstam equations were solved for the ππ-scattering s- and p-waves. To obtain resonance in the p-waves, it is necessary to cut off in these equations the left-half unphysical cut. We note that the left cut is cut off either very far ($\Lambda = 10^8$ [4]), or else the left cut is replaced by a far pole $\nu = -10^3$ [5]. Solutions were obtained with resonance only in the p-wave, due to the "bootstrap" mechanism. We shall show that such a resonance is determined by the contributions of large singularities of the left cut. [5]

Let us cut off the left cut in the Chew-Mandelstam equations

$$A_i(\nu) = \frac{1}{\pi}\int_0^\infty \frac{\operatorname{Im} A_i(\nu')}{\nu'-\nu}d\nu' + \frac{1}{\pi}\int_0^\Lambda \frac{f_i(\nu')}{\nu'+\nu+1}d\nu',$$

$$f_i(\nu) = \frac{1}{\nu+1}\int_0^\nu \left(1-2\frac{\nu'+1}{\nu+1}\right)\left[\alpha_{i0}\operatorname{Im} A_0(\nu') + \alpha_{i2}\operatorname{Im} A_2(\nu') + 3\left(1-2\frac{\nu}{\nu'}\right)\alpha_{i1}\operatorname{Im} A_1\right]d\nu'.$$

We shall show that the solutions with coinciding resonances in the s- and p-waves satisfy the Chew-Mandelstam equation for a small cutoff parameter.

We consider the δ-approximation

$$\operatorname{Im} A_1(\nu) = \lambda\pi\alpha_1\delta(\nu-\nu_r),$$

$$\operatorname{Im} A_0(\nu) = \lambda\pi\alpha_0\delta(\nu-\nu_r), \qquad \operatorname{Im} A_2(\nu) = 0.$$

Here $\lambda\alpha_i = \Gamma_i$, Γ_i is the total resonance width, and ν_r is the position of the coinciding resonances. Then

$$f_1(\nu) = \frac{\pi\lambda}{\nu+1}\left(1-2\frac{\nu_r+1}{\nu+1}\right)\left[\frac{2}{3}\alpha_0 + 3\left(1-\frac{\nu}{\nu_r}\right)\alpha_1\right].$$

The threshold condition of the p-wave yields

$$2\nu_r\frac{\lambda-\nu_r}{(\Lambda+1)^2}\alpha_0 = 3\alpha_1\left[1-6\ln\frac{\Lambda+1}{\nu_r+1} + 3(4\Lambda+2-\nu_r)\right]. \tag{1}$$

We put $\alpha_0 = \varphi(\Lambda)\alpha_1$; the function $\varphi(\Lambda)$ is shown in Fig. 1. At not too large values of Λ, this is the condition for the correlation between the A_0- and A_1-waves, and consequently, confining ourselves to low-energy contributions, we find that resonance in the p-wave is due to resonance of the A_0-wave.

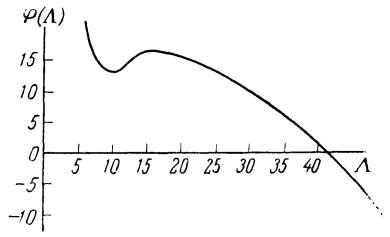

FIG. 1

For Λ >40 (energy ~ 2 BeV) the function $\varphi(\Lambda)$ becomes negative and there is no wave correlation. The A_0-wave satisfies the threshold condition independently of the A_1 wave; the resonance is produced by the "bootstrap" mechanism; it is impossible at low cut-off. When Λ = 10—15, condition (1) leads to an exact connection between α_0 and α_1 in Eqs. (3.8) of [1]:

$$\alpha_0 = 14\alpha_1.$$

Combining the threshold conditions with the normalization of the A_0 wave: $A_0(0) = 5\lambda$,

$$\alpha_0\left[1+\frac{2}{3}\nu_r\frac{\lambda-\nu_r}{(\Lambda+1)(\nu_r+1)}\right] + 6\alpha_1\left[\frac{\Lambda-\nu_r}{1+\Lambda}\frac{2+\nu_r}{1+\nu_r} - 2\ln\frac{\Lambda+1}{\nu_r+1}\right] = 5\nu_r, \tag{2}$$

we obtain the dependence of α_1 on Λ (see Fig. 2). For Λ = 10—15 we get $\alpha_1 = \Gamma_1/\lambda = 2.14$, Γ/λ