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F. Palumbo: BEHAVIOUR AT THE ORIGIN OF THE PARTIAL WAVES IN THE HYPERSPHERICAL EXPANSION OF MANY--PARTICLE WAVE FUNCTIONS.

Abstract: It is shown that the partial waves of the hyperspherical expansion of many-particle wave functions have only logarithmic singularities at the origin, provided the two-body potential is not more singular than r^{-2}.

The Schrödinger equation for a system of N particles interacting via a local potential is a partial differential equation in a 3N-dimensional space. After separation of the c. m. coordinates, it reduces to a partial differential equation in a 3(N-1) dimensional space for the intrinsic motion. Introducing the hyperradius ϱ and a set of 3N-4 angular coordinates this partial differential equation can be transformed[(1)] into an infinite system of ordinary differential equations in ϱ, by a procedure very close to that used in the three-dimensional case, where ordinary polar coordinates are used:

$$\left(\frac{d^2}{d\varrho^2} - \frac{\mathscr{L}_K(\mathscr{L}_K+1)}{2} + E\right)\chi_{K\gamma_K} - \sum_{K'\gamma_{K'}} W_{K\gamma_K, K'\gamma_{K'}} \chi_{K'\gamma_{K'}} = 0 \qquad (1)$$

Here $\mathscr{L}_K = K + \frac{3N-6}{2}$, $K = K_m, K_m+2, \ldots$, the minimum value of K, K_m, depending on the statistics of the particles[1], while γ_K ranges in a domain D_K which need not be specified here. The functions $\chi_{K\gamma_K}(\varrho)$ are often called partial waves. The knowledge of the behaviour at the origin of the partial waves can be useful for the qualitative understanding of the structure of many-particle systems, in numerical computations and in the study of the asymptotics of form factors. Such a behaviour has already been established[2] for the case where the two-body potential is more singular than r^{-2}. In this paper we will consider the case of two-body potentials behaving like r^{-n}, with n integer, and will derive in detail the behaviour of the partial waves at the origin for $n < 2$, while the marginal case of $n=2$ will only be sketched at the end. Our results will actually be established for the solutions of system (1) truncated at an arbitrary finite value of K, say K_M, and nothing will be said about the convergence of such solutions for $K_M \longrightarrow \infty$.

We first rewrite eqs. (1) in the vector-matrix form[3]

$$\left[\varrho^2 \frac{d^2}{d\varrho^2} - \mathscr{L}(\mathscr{L}+1) - A\right]\chi = 0, \qquad (2)$$

by introducing the column vector χ with components $\chi_{K\gamma_K}$, and the matrices

$$\mathscr{L}_{K\gamma_K, K'\gamma_{K'}} = \mathscr{L}_K \delta_{KK'} \delta_{\gamma_K \gamma_{K'}} \qquad (3)$$

$$A_{K\gamma_K, K'\gamma_{K'}} = \varrho^2 (W_{K\gamma_K, K'\gamma_{K'}} - E\,\delta_{KK'}\delta_{\gamma_K\gamma_{K'}}). \tag{4}$$

The number of eq. (2) is $\frac{K_M - K_m}{2} + 1$, so that there are $K_M - K_m + 2$ linearly indipendent solutions. Only half of them, those regular at the origin, are physically meaningful and we shall lable them $\chi^{(K\gamma_K)}$. We will ignore the irregular solutions.

For a reason which will become clear later we define a one-parameter family of vectors $\Lambda^{(K\gamma_K)}(\sigma, \varrho)$ depending on the parameter σ. The matrix A and the vectors $\Lambda^{(K\gamma_K)}(\sigma, \varrho)$ can be formally expandend in power series

$$A = \sum_{\nu=0}^{\infty} A_\nu \varrho^\nu, \tag{5}$$

$$\Lambda^{(K\gamma_K)}(\sigma,\varrho) = \varrho^{\mathscr{L}_K + 1 + \sigma} \sum_{\nu=0}^{\infty} \Phi_\nu^{(K\gamma_K)}(\sigma)\varrho^\nu, \tag{6}$$

where

$$\Phi_0^{(K\gamma_K)}(\sigma) = \sigma^{\frac{K_M - K_m}{2}} E^{(K\gamma_K)};\quad E_{K'\gamma_{K'}}^{(K\gamma_K)} = \delta_{KK'}\delta_{\gamma_K\gamma_{K'}}, \tag{7}$$

and for $\nu > 0$ the $\Phi_\nu^{(K\gamma_K)}(\sigma)$ are defined by the recursion formulae

$$\left[(\mathscr{L}_K + \sigma + \nu)(\mathscr{L}_K + 1 + \sigma + \nu)I - \mathscr{L}(\mathscr{L}+1)\right]\Phi_\nu^{(K\gamma_K)}(\sigma) = \\ = \sum_{\mu=0}^{\nu} A_\mu \Phi_{\nu-\mu}^{(K\gamma_K)}(\sigma), \tag{8}$$

where I is the unit matrix, $I_{K\gamma_K, K'\gamma_{K'}} = \delta_{KK'}\delta_{\gamma_K\gamma_{K'}}$.

We now use our restriction that the two-body potential should behave like r^{-n} at the origin, with n integer less than 2. Due to the fact [1] that the functions $W_{K\gamma_K, K'\gamma_{K'}}$ of eq. (4) behave at the origin as functions of ϱ as the two-body potential as a function of r, we have $A_\nu = 0$ for $\nu \leq 1-n$, so that $A_o = 0$ for $n < 2$. Eq. (8) can then be rewritten

$$\left[(\mathscr{L}_K+\sigma+\nu)(\mathscr{L}_K+1+\sigma+\nu)\mathrm{I} - \mathscr{L}(\mathscr{L}+1)\right] \Phi_\nu^{(K\gamma_K)}(\sigma) = \sum_{\mu=o}^{\nu-1} A_{\mu+1} \Phi_{\nu-\mu-1}^{(K\gamma_K)}(\sigma). \tag{9}$$

For $0 < |\sigma| < 2$ the elements of the diagonal matrix in the square brackets in eq. (9) never vanish so that eq. (9) can actually be solved with respect to the $\Phi_\nu^{(K\gamma_K)}(\sigma)$, which is the reason why the parameter σ has been introduced. Ita can be shown [3] that the series (6) so defined converges uniformly both with respec to σ and ϱ in a neighborood of $\varrho = 0$, and it is easy to verify that it satisfies the inhomogeneous vector-matrix differential equation

$$\left[\varrho^2 \frac{d^2}{d\varrho^2} - \mathscr{L}(\mathscr{L}+1) - A\right] \Lambda^{(K\gamma_K)}(\sigma,\varrho) = \left[(\mathscr{L}_K+\sigma)(\mathscr{L}_K+1+\sigma)\mathrm{I} - \mathscr{L}(\mathscr{L}+1)\right] \sigma^{\frac{K_M-K_m}{2}} E^{(K\gamma_K)}. \tag{10}$$

We can now state our result: the set of independent solutions regular at the origin is

$$\chi^{(K\gamma_K)}(\varrho) = \lim_{\sigma\to o} \frac{d^{\frac{K_M-K_m}{2}}}{d\sigma^{\frac{K_M-K_m}{2}}} \Lambda^{(K\gamma_K)}(\sigma,\varrho) = \varrho^{\mathscr{L}_K+1} \sum_{\tau=o}^{\frac{K_M-K_m}{2}} (\ln\varrho)^\tau \varphi_\tau^{(K\gamma_K)}(\varrho), \tag{11}$$

where

$$\varphi_{\tau}^{(K\gamma_K)}(\varrho)=\frac{\left(\frac{K_M-K_m}{2}\right)!}{\tau!\left(\frac{K_M-K_m}{2}-\tau\right)!}\lim_{\sigma\to o}\frac{d^{\frac{K_M-K_m}{2}-\tau}}{d\sigma^{\frac{K_M-K_m}{2}-\tau}}\sum_{\nu=o}^{\infty}\Phi_{\nu}^{(K\gamma_K)}(\sigma)\,\varrho^{\nu}. \tag{12}$$

That these functions are actually solutions can be verified by taking the $\frac{K_M-K_m}{2}$-th derivative with respect to σ of both sides of eq. (10). The rigth hand side vanishes in the limit $\sigma \longrightarrow 0$ and being $\frac{d}{d\sigma}$ parmutable with $(\varrho^2\frac{d^2}{d\varrho^2}-\mathscr{L}(\mathscr{L}+1)-A)$, $\chi^{(K\gamma_K)}(\varrho)$, given by eq. (11) is indeed a solution of eqs.(1). Moreover, being the $E^{(K\gamma_K)}$ independent vectors, the $\chi^{(K\gamma_K)}(\varrho)$ are independent .

It only remains to display the structure of the solutions we have found. All the $\Phi_{\nu K'\gamma_{K'}}^{(K\gamma_K)}(\sigma)$ are olomorphic functions of σ . $\Phi_o^{(K\gamma_K)}(\sigma)$ has a zero of order $\frac{K_M-K_m}{2}$ at $\sigma = 0$, which is taken cure of by the $\left(\frac{K_M-K_m}{2}\right)$-th derivative with respect to σ , so that in the limit $\sigma \longrightarrow o$ $\Psi_o^{(K\gamma_K)}(\sigma)$ is finite. The same for $\nu = 1$. For $\nu = 2$ something new happens, because the diagonal matrix in the left-hand side of eq. (8) has a simple zero at $\sigma = 0$, so that $\Phi_2^{(K\gamma_K)}(\sigma)$ has a zero of order $\frac{K_M-K_m}{2}-1$ at $\sigma=0$, and a logarithmic factor originates from the differentiation of $r^{\mathscr{L}_K+1+\sigma+2}$

$\Phi_3^{(K\gamma_K)}(\sigma)$ also has a zero of order $\frac{K_M-K_m}{2}-1$, so that only one logarithmic factor is present, but $\Phi_4^{(K\gamma_K)}(\sigma)$ has a zero of order

$\frac{K_M-K_m}{2}-2$, so that two logarithmic factors are generated by differentiation. The power $(\ln\varrho)^{\frac{K_M-K_m}{2}}$ will appear with $\Phi^{(K\gamma_K)}_{\frac{K_M-K_m}{2}}(\sigma)$ and there will be no higher powers of ln ϱ. We stress that the appearence of such logarithmic factors is unavoidable with the exception of the solution vector $\chi^{(K_M\gamma_{K_M})}$ which has no logarithms, due to the fact that the elemens of the diagonal matrix in square brackets in eq. (9) never vanish even for $\sigma=0$ for this solution. It follows from the above discussion that

$$\varphi^{(K\gamma_K)}_{oK'\gamma_{K'}}(\varrho)=\left(\frac{K_M-K_m}{2}\right)!\,\delta_{KK'}\delta_{\gamma_K\gamma_{K'}}+\varrho\lim_{\sigma\to o}\frac{d^{\frac{K_M-K_m}{2}}}{d\sigma^{\frac{K_M-K_m}{2}}}\Phi^{(K\gamma_K)}_{1K'\gamma_K}(\sigma)+\ldots \tag{13}$$

showing that the component $(K\gamma_K)$ of the vector $\chi^{(K\gamma_K)}(\varrho)$ behaves like $\varrho^{\mathscr{L}_K+1}$ as in the absence of interaction. According to eq. (9) all the other components behave like $\varrho^{\mathscr{L}_K+2+1-n}$, depending on the two-body potential.

For $\tau>0$ and $n=1$ the leading component of the vector $\varphi^{(K\gamma_K)}_{\tau}(\varrho)$ is

$$\varphi^{(K\gamma_K)}_{\tau,K+2,\gamma_{K+2}}(\varrho)\sim\varrho^{2\tau}, \tag{14}$$

while all the other components behave like $\varrho^{2\tau+1}$. It is easy to find the analogous result for $n < 1$.

We conclude by sketching the procedure to be used for potentials behaving like r^{-2} at the origin. In such a case the matrix $A_o \neq 0$. We must then replace the $\chi^{(K\gamma_K)}(\varrho)$ by those linear superpositions which diagonalize the matrix $\mathscr{L}(\mathscr{L}+1)+A_o$, which can be done because A_o is hermitean. We come in this way into a situation similar to the one we have treated in detail.

The problem of stability of the system of particles, that in such a case arises can be discussed along the same line as in the two-particle case treated by Landau and Lifschitz[(4)].

The above treatment encompasses the deuteron problem for the coupled s-d channels. In such a case the system (1) contains only two equations with $\mathscr{L}_{K_m}=0$ and $\mathscr{L}_{K_M}=2$.

The possible occurrence of logarithms as well as the modification of the behaviour of the partial waves with respect to the uncoupled case were already mentioned in the literature[(5)] for such a case, but no detailed derivation is known to the author. Such a detailed derivation is contained in the above. For Yukawa potentials, for instance, the S and D partial waves behave like r^0 and r^1 for the lower energy solution, and like r^3 and r^2 for the higher energy solution resp. (the χ functions of eqs. (1) have one additional power of r).

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