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SOME MATHEMATICAL ASPECTS OF THE STURM-LIOUVILLE EXPANSION WITH SPECIAL REFERENCE TO THE NUCLEON-NUCLEUS POTENTIAL. II

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Некоторые математические вопросы метода разложения по функциям Штурма-Лиувилля в задачах ядерной физики. II .

Исследованы различные свойства сходимости разложений по функциям Штурма-Лиувилля, причём особое внимание уделено уравнениям типа уравнения Шредингера с фиксированной энергией и с потенциалами различной глубины, в частности, с потенциалом Саксона-Вудса, широко используемого в ядерной физике. Метод обобщен для многомерного случая и показано, что полученные волновые функции могут быть применены для вычисления сечения прямых ядерных реакций между сложными ионами. Полнота используемого базиса делает этот метод предпочтительным перед другими методами разложения и дает возможность проконтролировать точность полученных результатов. В частности, для функций, удовлетворяющих уравнению Шредингера с потенциалом, который уменьшается с увеличением расстояния r, показано, что сходимость полученных рядов не слабее, чем n^{-4}.

Работа выполнена в Лаборатории теоретической физики ОИЯИ и в Институте Нильса Бора.

Сообщение Объединенного института ядерных исследований. Дубна 1977

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Some Mathematical Aspects of the Sturm-Liouville Expansion with Special Reference to the Nucleon-Nucleus Potential. II.

Different covergence properties of the Sturm-Liouville expansion are investigated with particular attention to the case of states which satisfy Schrödinger-like equations with a fixed energy and different depths of a potential, particularly of the Woods-Saxon shape used in nuclear physics.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR and Niels Bohr Institute.

Communication of the Joint Institute for Nuclear Research. Dubna 1977

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Introduction

In a recent publication, henceforth referred to as A (we used common numeration in the formulas), some convergence problems of Sturm-Liouville expansions were considered, with particular regard to nuclear physics problems. In this paper, some remaining questions are elucidated. In order to understand the importance of the different terms in calculations of physical properties, a knowledge of the shape of the SL-functions, as well as of their eigenvalues, is necessary. This is provided in Section (V).

The solutions of three-dimensional problems are in (VI) shown to possess convergence properties for $r \to \infty$, which are similar to those found in A for the one-dimensional problem.

The problems considered up to this point can be called one-body problems with fixed potentials, or two-body problems in relative coordinates. In (VII) we consider the problems of more particles, for the special case, relevant to nuclear problems, that one is much heavier than the others. It is shown, that the asymptotic behaviour of this system is rather complicated, but that nevertheless, in some important cases, it is possible to approximate the form factor well by an SL-expansion.

In (VIII) we give examples, suited to illustrate some of the statements of the earlier sections.

V. The Sturmian functions and eigenvalues

Since the pure Coulomb potential, used in atomic physics, has well known analytic solutions and eigenvalues (charges) of the SL problem, we shall here limit ourselves to consideration of the spherical Woods-Saxon potential. The case of combined nuclear attraction and Coulomb repulsion is of equal interest, and is very similar to the pure nuclear case in all relevant respects.

The fundamentals of the theory of the solutions and eigenvalues of eq. (3) A is the Sturmian fundamental theorem, which for our purpose can be stated as follows.

Given two functions, f_1 and f_2 which satisfy

$$-f_1''(r) + (u_1 - E) f_1(r) = 0 \tag{76}$$

and

$$-f_2''(r) + (u_2 - E) f_2(r) = 0$$

respectively, and in a given interval

$$R \le r \le S \ , \quad u_1(r) > u_2(r) \ . \tag{77}$$

Then, between two consecutive zeroes of f_1 there will be at least one of f_2.

This follows from

$$[f_1' f_2 - f_2' f_1]_{r_1}^{r_2} = \int_{r_1}^{r_2} (u_1 - u_2) f_1 f_2 \, dr. \tag{78}$$

Let r_1, r_2 be consecutive zeroes of f_1 and suppose that there is no zero of f_2 in (r_1, r_2), then we may, without lack of generality, assume both functions to be positive in (r_1, r_2).

Then $f_1'(r_1) \geq 0$, $f_1'(r_2) < 0$, so the left-hand side of equation (78) is negative and the right is positive, i.e., a contradiction, which is removed only because the assumption of no zero of f_2 was false.

If we now consider equation (3) A with the boundary condition $f(0) = 0, (f'(0) \neq 0)$ and let λ grow, we see that the number of zeroes is a never decreasing function of λ , that all zeroes move towards smaller r -values, and that new zeroes therefore must start at infinity, when λ is an eigenvalue. A zero, born in an internal point would have to be born as double, but double zeroes are excluded by eq. (3) A and the boundary conditions[2]. We can say, that with larger λ the solutions become more and more oscillating. The eigensolutions are of course oscillating only in the regions, where $E - \lambda V - V_0 > 0$ (Now, looking only at the radial equation, we will let V_0 include the centrifugal barrier).

If we introduce the new coordinate

$$x = \int_0^r \left(-V(r')\right)^{1/2} dr' \tag{79}$$

we see, that with the potentials introduced here, the function

$$h_i = (-V)^{1/4} f_i \tag{80}$$

will satisfy an equation

$$\frac{d^2}{dx^2} h_i + \left(\lambda_i + U(x)\right) h_i = 0 \tag{81}$$

and that the infinite interval $0 \leq r \leq \infty$ is transformed into a finite interval $0 \leq x \leq b$ the normalization becoming

$$\int_0^b dx\, h_i^2(x) = 1. \tag{82}$$

Using the proof of Ref. 2, we then see, that h_i is always below some limit, independent of i and x. The same must therefore be the case with

$$g_i = (-V)^{1/2} f_i = (-V)^{1/4} h_i \qquad (83)$$

independent of i and r.

Sturm's fundamental theorem can also be used to estimate the eigenvalues. First, it is clear from the above, that with given ℓ, j , the nth eigenfunction, corresponding to the radial quantum number n, has n modes. In order to simplify matters we shall neglect the spin orbit-coupling which anyway is not very important. Now, the Woods Saxon potential (3) A lies totally below the potential

$$U_1 = \infty \quad \text{for} \quad r > R - a$$

$$U_1 = -\frac{\lambda}{1+\exp(-1)} = -0.27\lambda \quad \text{for} \quad r \leq R - a \,. \qquad (84)$$

For $r < R_\ell$

$$-\frac{\lambda}{1+\exp\frac{R_\ell - R}{a}} + \frac{\ell(\ell+1)}{R_\ell^2} + E_B = 0 \quad (E_B = -E > 0) \qquad (85)$$

the Woods Saxon potential (3) A lies above the potential

$$U_\ell = -\lambda \,, \qquad U_\ell = \infty \qquad (86)$$

for $r > R_\ell$, there are no zeroes of $f(\lambda)$.

For $\ell = 0$, the solutions of the SL equation with U_1 and U_2 are just sin ($\varkappa r$) with

$$\varkappa_1^2 = 0.27\lambda - E_B \qquad (87)$$

and

$$\varkappa_\ell^2 = \lambda - E_B \qquad (88)$$

respectively,

so the number of zeroes n_1 , n_ℓ is in the two cases given by

$$x_1(R-a) = (n_1 + \nu_1)\pi \quad , \quad 0 \le \nu_1 < 1 \tag{89}$$

$$x_\ell R_{(\ell=0)} = (n_\ell + \nu_\ell)\pi \quad , \quad 0 \le \nu_\ell < 1 \tag{90}$$

respectively, or

$$\pi^{-\ell}(n_1+\nu_1)^{\ell}(R-a)^{-\ell} + E_B = 0.22\lambda \tag{91}$$

$$\pi^{-\ell}(n_\ell+\nu_\ell)^{\ell}\left(R + a\ln\left(\frac{\lambda}{E_B} - 1\right)\right)^{-\ell} + E_B = \lambda \ . \tag{92}$$

We see from (91), that λ has no upper limit. Since we know, that λ_n is a monotonous function of n this should mean, that we can find n-values, so that λ_n can be larger than any given number, e.g., $2E_B$. But then we see from (91) and (92), that

$$\pi^{-\ell} n^{\ell} R^{-\ell} + E_B < \pi^{-\ell} n^{\ell}\left(R + a\ln\left(\frac{\lambda}{E_B} - 1\right)\right)^{-\ell} + E_B$$
$$< \lambda_n < \left(\pi^{-\ell}(n+1)^{\ell}(R-a)^{-\ell} + E_B\right)/0.22 . \tag{93}$$

For $\ell \neq 0$, an estimate of the number of zeroes for the two potentials U_1 and U_2 can be obtained from the relation between the zeroes of j belonging to ℓ and $\ell-1$

$$j_{n,\ell-1} < j_{n,\ell} < j_{n+1,\ell-1} \ , \tag{94}$$

where j_ℓ are Bessel functions.
So , the position of the n'th zero is subjected to the inequalities

$$j_{n,0} < j_{n,\ell} < j_{n+\ell,0} . \tag{95}$$

Consequently, for the number of zeroes we have in the two cases corresponding to (84) and (86), respectively:

$$\begin{aligned} n_1 > n > n_1 - \ell \\ n_\ell > n > n_\ell - \ell . \end{aligned} \tag{96}$$

Since the number of zeroes is identical to the radial quantum number, n (or, according to another definition, n-1), we see that for large n we have, in all cases,

$$\lambda_{n,\ell} = C_\ell \, n^2 + O(n) . \tag{97}$$

It follows directly from Sturm's fundamental theorem that the eigenvalues $\lambda_{n,\ell}$ for ℓ fixed and different n, are non-degenerate.

As the radial equation with a Woods-Saxon potential, in the case of $\ell = 0$ can be transformed into a hypergeometric equation, we know the spectum, which is actually similar to that of a square well, also for small n-values. So it is far from degeneracy, and the same is actually the case for $\ell \neq 0$.

But the feature of being far from degeneracy is particular for the spectrum of the one-dimensional (radial) equation. If we look at the many-particle case, we should,of course, expect the same degeneracies as with E-values, but already with one particle moving, e.g., in a spherical potential, we must expect that $\lambda_{n,\ell}$'s belonging to different ℓ-values can lie near each other, as we shall see in the next section.

VI. Three-dimensional problems

The radial equation of the Woods-Saxon potential, with or without a Coulomb term, must, apart from the above-mentioned case, be solved numerically. Any additional radial potential would therefore most simply be included directly in the numerical calculation.

The utility of the SL-method lies in its application to multi-dimensional calculations, and the one-dimensional examples given above, are only meant as illustrations of the problems met in the latter cases.

We shall here concentrate upon the two cases met in the literature of nuclear problems, namely of one particle interacting with a static or oscillating deformed field, and of several particles interacting with each other, as well as with the nuclear (+ Coulomb) potential.

As mentioned above, one main difference with the one-dimen-

sional case is that we must now expect degeneracy to exist. If we specially think of the spherical one-particle orbits, we must expect that for given E, $\lambda_{n,\ell}$ values corresponding to the same value of $2n+\ell$ must lie near each other. The reason is evidently the similarity between the Woods-Saxon-potential and that of a harmonic oscillator, where such a degeneracy is complete. The very similar near-degeneracy of E-values in usual shell model calculations is well-known, only we see now that with the λ - values, the same phenomenon is found with much higher quantum numbers, too.

This approximate degeneracy will, of course, exclude the general use of perturbation theory to the problems we are considering. At least, the degeneracy must first be lifted by direct diagonalisation of the Hamiltonian, including residual interactions. Only for small admixtures of SL components with λ_i very different from the λ of the Hamiltonian ($\gamma=1$ in equation (50), etc.) perturbation theory, such as sketched in section IV in A, is applicable[3,4]. This does not contradict the general arguments of that section, based on the smallness of coefficients of the order

$$C_i = \frac{\sigma_{i0}}{\lambda_i - \lambda_0} \tag{98}$$

for very high i-values.

As for the special convergence properties, discussed in section III, they will in general be shared by the 3-dimensional solutions, with very similar restrictions on potentials and interaction. The proofs are more complicated, and we shall only sketch how to find sufficient conditions for the uniform convergence of the logarithm.

Let us assume all f_n and f to be real, and let us define

$$\rho = \begin{cases} \rho_\alpha = \dfrac{f_N(r)}{f(r)} & \text{for } |f_N(r)| \leq |f(r)| \\ \rho_\beta = \dfrac{f(r)}{f_N(r)} & \text{for } |f_N(r)| \geq |f(r)| \end{cases} \tag{99}$$

We can now draw surfaces of constant ρ, σ_ρ and curves perpendicular to those s, following grad $\rho(r)$. The differential equations, satisfied by f and f_n, ensure the possibility of

this construction. A closed curve, t, on a σ defines a surface segment ω_σ, and the s, intersecting σ in t, define the surface, τ, of a "tube". Proceeding further away from σ, τ must either narrow down, ending at an extremum point of P, or it may end in an extremal curve, or go to infinity. In the two latter cases, it is possible to close the tube by a surface, τ' on which either, like on τ, the surface integral

$$\int_{\tau'} d\sigma (f \nabla f_N - f_N \nabla f) = \begin{cases} \int_{\tau'} d\sigma f^2 \nabla p_\alpha \\ \int_{\tau'} d\sigma f_N^2 \nabla p_\beta \end{cases} \qquad (100)$$

is exactly zero, or, in the case of τ' stretching to infinity, can be made arbitrarily small. It should be noticed, too, that the integrand obviously has no singularities.

On the "tube", t, closed in this way, we can now use Green's theorem

$$\int_{\tau+\tau'+\omega} d\sigma (f \nabla f_N - f_N \nabla f) = \int_{\omega} d\sigma (f \nabla f_N - f_N \nabla f) + \delta$$

$$= \int_t d\underline{r} (f \Delta f_N - f_N \Delta f) = \int_t d\underline{r} (h_N V - f_N V_1) f, \qquad (101)$$

where h_N is defined as in (33)A. We can now again make the assumption (31)A and, proceeding as before, we see that if (36)A is replaced by

$$\left| \int_t d\underline{r} \, |V(\underline{r})| \, f^{1/2}(\underline{r}) \right| < C_2 f^2(\omega_\sigma) K(\omega_\sigma) \omega_\sigma \qquad (102)$$

we can prove the smallness of ∇p_α or ∇p_β in the respective cases on the surface segment ω_σ if this was chosen so that p had one sign on it. Here $K(\omega_\sigma)$ is a slowly varying function of space, say

$$K(\omega_\sigma) = r_\omega^{-\gamma}, \quad \gamma > 1 \qquad (103)$$

which ensures that also the curve integral

$$\left| \int d\bar{r} \nabla p \right| < \eta \qquad (104)$$

for any curve, thus leading to the desired convergence.

It is seen that with V being of the Woods-Saxon type (3)A, and V_1 being the deformation term, given, e.g., as

$$V(r - R(\Omega)) - V(r - R)$$
$$R(\Omega) = R\left(1 + \sum_{\ell m} \beta_{\ell m} Y_{\ell m}(\Omega)\right) \qquad (105)$$

or any of the other expressions, which have been suggested in the literature[5], (31) and (102) are fulfilled, again by the condition of $2\varkappa a < 1$.

What has been said here concerns, stricly speaking, the extreme adiabatic case, where the coupling to the deformed field is that to a completely inert core. This is to a high accuracy fulfilled in rotational states of deformed nuclei. If we go to vibrational cores, the coupling is of the same type, but it connects states of different binding energy, which means that, in principle, different Sturmian bases must be introduced for different components of the wave function[6] (but only one basis for each form factor). The important feature of finite range of the potential, as well as the residual interactions, is however still at hand, so we must expect the convergence features to be essentially the same as above.

In the discussion above, we have made no assumptions concerning the shape of the potential or residual terms, even the number of dimensions could presumably easily be changed. In practical calculations we have, however, always resorted to the 3-dimensional equation with V being spherical, the calculational advantages and applicability of this basis being obvious.

VII. Problems with several particles

In the case of more particles, not only the equations, but even the asymptotic behaviour is, as we shall see below, more complicated than for one, and instead of reproducing it exactly, we shall discuss the possibility of obtaining a satisfactory compromise between this and the requirements for a simple wave function.

We shall only discuss the case of two identical particles, interacting with each other and with an inert core. The guiding physical idea is here the relative weakness of the interaction between the particles, and particularly the fact that no bound system of two like particles exists.

We shall consider the inert core as infinitely heavy, corresponding, approximately, to the physical system of two identical particles outside a very heavy closed shell core, like ^{208}Pb.

We shall neglect spins and Coulomb forces, thus looking at the solutions of

$$\left(H_0 + \lambda^{(1)} V(r_1) + \lambda^{(2)} V(r_2) + \gamma V_{12}(|\underline{r}_1 - \underline{r}_2|) - E \right) \Psi = 0. \quad (106)$$

The generalization to a genuine three-body problem with, e.g., three interacting nucleon is straightforward, and the SL expansion was actually shown in a numerical way, by J.P.Boisson and C.Gignoux[7], to converge rather fast for a number of such cases.

However, already with the above-mentioned model, which is in a way the simplest possible many-particle system, we meet the problem of the complicated structure of the wave function for large values of r_1 and r_2.

The general asymptotic form of bound three-body-wave-functions was studied by S.P.Merkuriev[8] and we shall, without repeating his proofs, lean on his results, which are simplified somewhat in the above-mentioned case.

We shall make the further assumption that the state has parentage to one state of the system of core-plus-one particle only, this state having the binding energy

$$-E_1 = \varkappa_1^2 \quad (107)$$

The binding energy of the two particle state will be denoted

$$E_2 = -E = \varkappa^2 . \quad (108)$$

Now, we divide the 6-dimensional configuration space of our problem into three regions

a) $r_2^2 (E_2 - E_1) < r_1^2 E_1$

b) $r_1^2 E_1 < r_2^2 (E_2 - E_1)$, $r_2^2 E_1 < r_1^2 (E_2 - E_1)$ (109)

c) $r_1^2(E_2-E_1) < r_2^2 E_1$.

Then the asymptotic shape of the wave function in each of the 3 regions

$$\text{a)}\ \frac{1}{r_1 r_2}\exp\left(-\varkappa_1 r_2 - (\varkappa^2-\varkappa_1^2)^{1/2} r_1\right)$$

$$\text{b)}\ \frac{1}{r^{5/2}}\exp(-\varkappa r)\ ,\quad r^2 = r_1^2+r_2^2 \qquad (110)$$

$$\text{c)}\ \frac{1}{r_1 r_2}\exp\left(-\varkappa_1 r_1 - (\varkappa^2-\varkappa_1^2)^{1/2} r_2\right).$$

The apparent difference in dimensionality of the expressions (110, a), c)) and (110, b)) should lead to no confusion; it just corresponds to the use of different elements of space $r_1^2\, dr_1\, r_2^2\, dr_2\, d\Omega_1\, d\Omega_2$ and $r^5\, dr\, d\Omega$ in the two cases.

If a bound state of the two light particles had existed, there would have dominated the asymptotic behaviour in a fourth region, lying in the middle of region b. What is meant here by asymptotic shape, is the behaviour as a function of r_1, r_2, as r goes to infinity; in each region the function is further multiplied by an innocent function of the angles and of r_1/r_2.

The forms given by (110) are correct on five-dimensional surfaces of constant r; for surface of smaller dimensionality with r given, other shapes must be envisaged. Particularly, on the borders between a) and b) and between b) and c), the shape is an error function of r. For $r_1 \to 0$ or $r_2 \to 0$ we get, in these variables, respectively, bound state wave functions in the potential V. A special interest is further presented by the surface $r_1 = r_2$, which we consider more closely below.

Even looking apart from these surfaces of measure zero, compared to the first ones, we see that the asymptotics is too complicated for the construction of completely appropriate SL functions. A simple SL basis could be found for each of the three asymptotic shapes, a) or b) or c), but no simple basis functions could share all three asymptotic forms.

In practice, however, we may use the fact that in the most important cases, the extra binding energy due to the interaction

between the particles is positive, but much smaller than the total binding energy

$$x^2 = 2(x_1^2 + x'^2)$$
$$0 < x'^2 << x^2 . \tag{111}$$

We now introduce a set of functions with the asymptotic behaviour given by

$$\psi \sim \frac{1}{r_1 r_2} \exp(-x_h(r_1 + r_2))$$
$$x_h^2 = \frac{x^2}{2} . \tag{112}$$

Now the proportion between the asymptotics as given by (112) and the correct one is, approximately, in the three regions

a) $$a_a \sim \exp(r_2(x_1 - x_h) + r_1((x^2 - x_1^2)^{1/2} - x_h)) \simeq \exp\frac{x'^2}{2x_1}(r_1 - r_2) \tag{113}$$

b) $$a_\beta \sim \exp((-(r_1 + r_2) + (2(r_1^2 + r_2^2))^{1/2})(x_1^2 + x'^2)^{1/2})$$

c) $$a_c \sim \exp(r_1(x_1 - x_h) + r_2((x^2 - x_1^2)^{1/2} - x_h)) \simeq \exp\frac{x'^2}{2x_1}(r_2 - r_1) .$$

The form (113b) is valid, approximately, for

$$1 - \frac{2x'^2}{x_1^2} < \frac{r_2}{r_1} < 1 + \frac{2x'^2}{x_1^2} . \tag{114}$$

If we introduce $r' = r_2 - r_1$, the three proportions are

$$a_a \sim a_c \sim \exp\left(r' \frac{x'^2}{2x_1}\right)$$
$$a_\beta \sim \exp\left((x_1^2 + x'^2)^{1/2} \frac{r'^2}{4r_1}\right) \simeq \tag{115}$$
$$\exp\left((x_1^2 + x'^2)^{1/2} \frac{x'^2}{x_1^2} \frac{r'}{2}\right) \simeq \exp\left(r' \frac{x'^2}{2x_1}\right)$$

So we see that for small values of $\varkappa'$, the tail wave function is overestimated by using (112), by a factor $\leq \exp(r'\varkappa'^2/2\varkappa_1)$.

In practice, say, looking at the overlap factor (^{208}Pb, ^{210}Pb (g.s.)), we get

$$\frac{\varkappa'^2}{\varkappa_1^2} \sim 0.1, \quad \varkappa_1 \sim 0.5\ fm^{-1}$$

which means that for $r' \geq 10$ fm, the overestimate is about 25%. It is not likely that any transfer amplitude should get appreciable contributions from $r' \geq 10$ fm. For the simultaneous transfer the overestimate is even much smaller.

The asymptotic expression (112) defines a set of SL functions, which are products of functions, satisfying

$$(-\Delta + \lambda_i V - \varkappa_k^2) f_i = 0. \tag{116}$$

We could, of course, also have chosen a product of two sets, satisfying

$$\begin{aligned} (-\Delta_1 + \lambda_i V - (\varkappa^2 - \varkappa_1^2)) f_i(r_1) &= 0 \\ (-\Delta_2 + \lambda_j V - \varkappa_1^2) f_j(r_2) &= 0. \end{aligned} \tag{117}$$

This gives the correct asymptotic behaviour in region a) but not in c). In order to have this also, and to construct properly antisymmetrized wave-functions, we must then add a set of functions, satisfying the same equations with r_1 and r_2 permuted. Then, however, no orthogonality relation between functions belonging to different sets can be found, and still region b) would require a set of functions of quite another type.

Physical reasons will let some regions of space be more important than others, and in this respect, the above-mentioned regions of measure zero play a certain role. In one particle-transfer we probe, e.g., the region of small r_2 and arbitrary r_1. For such a calculation the basis given in (117) seems ideal, still, however, properly antisymmetrized. The error of using (112) will asymptotically be

$$\exp\left(-\frac{x'^2}{\ell x} r\right) \quad , \; r = r_1 \text{ or } r_2 \tag{118}$$

meaning in the above example that the proportion would drop by 25% when r increases by 10 fm. For small values of r_1 or r_2, where the oscillating part of the SL functions is probed, the dependence on x' is negligible, particularly when the basis is moderately large.

Thus taking into account the possibility of the energies being different with the basis sets $\{f^{(1)} f^{(2)}\}$ given by

$$\begin{aligned} (H_{01} + \lambda_n^{(1)} V^{(1)} - \varepsilon_1) f_n^{(1)} &= 0 \\ (H_{02} + \lambda_m^{(2)} V^{(2)} - \varepsilon_2) f_m^{(2)} &= 0 \; , \end{aligned} \tag{119}$$

expanding

$$\Psi_i(r_1, r_2) = \sum_{mn} c_{mn}^{(i)} f_n^{(1)} f_m^{(2)} \tag{120}$$

and inserting this in (106), we may either multiply from the left by $f_K^{(1)*} f_\ell^{(2)*}$ and integrate to obtain

$$\begin{aligned} &\sum_{mn} \left[(\varepsilon_1 + \varepsilon_2 - E) \langle K\ell | mn \rangle + \delta \langle K\ell | V_{12} | mn \rangle \right. \\ &\left. - (\lambda^{(1)} - \lambda_m^{(1)}) \langle \ell | n \rangle_2 \delta_{Km} - (\lambda^{(2)} - \lambda_n^{(2)}) \langle K | m \rangle_1 \delta_{n\ell} \right] c_{mn} = 0 \end{aligned} \tag{121}$$

or, before integration, multiply with $V^1 V^2 f_k^{(1)} f_\ell^{(2)}$ to get

$$\begin{aligned} &\sum_{mn} \left[(\varepsilon_1 + \varepsilon_2 - E) \delta_{Km} \delta_{n\ell} + \delta \langle K\ell | V^{(1)} V^{(2)} V_{12} | mn \rangle \right. \\ &\left. - (\lambda^{(1)} - \lambda_m^{(1)}) \delta_{\ell n} \langle K | V^{(1)2} | m \rangle_1 - (\lambda^{(2)} - \lambda_n^{(2)}) \delta_{Km} \langle \ell | V^{(2)2} | n \rangle_2 \right] c_{mn} = 0 \end{aligned} \tag{122}$$

where, by $\langle \ell | n \rangle$ the usual overlap $\int f_\ell^* f_n \, d\tau$,etc. is meant.

Now we meet the problem of choosing between the different diagonalization methods, as described in section IV.

Both equations can be put into the form

$$\{ E\underline{\underline{A}} + \lambda^{(1)}\underline{\underline{B}}_1 + \lambda^{(2)}\underline{\underline{B}}_2 + \gamma\underline{\underline{C}} + \underline{\underline{R}} \}\underline{C} = 0 , \qquad (124)$$

where $\underline{\underline{A}}$, $\underline{\underline{B}}_1$, $\underline{\underline{B}}_2$ and $\underline{\underline{C}}$ are Hermitian matrices.

However, $\underline{\underline{R}}$ is Hermitian only with (121) therefore though strong computational reasons should speak in favour of (122) the consideration of section IV leadsus to prefer (121), which can then, in 4 different ways, be considered as an eigenvalue problem, with eigenvalues E , $\lambda^{(1)}$, $\lambda^{(2)}$ or γ . Starting with a truncated set $\{ f^{(1)} f^{(2)} \}_N$ the diagonalization will in general give us a set of N independent functions

$$F_i = \sum_{mn}^{N} c_{mn}^{(i)} f_n^{(2)} f_m^{(1)} \qquad (125)$$

so that we obtain in this way SL-functions for the two-particle problem, which again form complete sets.

Even when all matrices $\underline{\underline{A}}$, etc., are Hermitian, the matrix which shall be diagonalized in order to obtain, e.g., E as an eigenvalue is not necessarily so:

$$E\underline{C} + \underline{\underline{A}}^{-1}\left(\lambda^{(1)}\underline{\underline{B}}_1 + \lambda^{(2)}\underline{\underline{B}}_2 + \gamma\underline{\underline{C}} + \underline{\underline{R}} \right)\underline{C} = 0 . \qquad (126)$$

In some important cases, it is nevertheless possible to transform (126) into a straightforward diagonalization problem. As an example, we may take the γ eigenvalue problem, which is important since $\lambda^{(1)}, \lambda^{(2)}$ may be said to be determined from the corresponding odd problems.

Consider $\underline{\underline{C}}$ given by (121), and let us write this as

$$\underline{\underline{C}} = \int g_k^{(1)*} g_\ell^{(2)*} \frac{V_{12}}{V^{(1)}V^{(2)}} g_m^{(1)} g_n^{(2)} d\tau_1 d\tau_2 . \qquad (127)$$

Now, if V_{12} has only one sign, we may always assume this to be positive, the sign of the interaction will then be the sign of γ . V^1V^2 will, as usual also be assumed to be positive everywhere. The (127) can, using the completeness relation for the g's, also be written

$$\underline{\underline{C}} = \sum_{st} \int g_u^{(1)*} g_e^{(2)*} \left(\frac{V_{12}}{V^{(1)}V^{(2)}}\right)^{1/2} g_s^{(1)} g_t^{(2)} d\underline{r}_1 d\underline{r}_2 \int g_s^{(1)*} g_t^{(2)*} \tag{128}$$

$$\left(\frac{V_{12}}{V^{(1)}V^{(2)}}\right)^{1/2} g_m^{(1)} g_n^{(2)} d\underline{r}_1' d\underline{r}_2' = \underline{\underline{C}}^{1/2} \underline{\underline{C}}^{1/2}$$

and, instead of (126), or its equivalent for γ, we obtain

$$\left\{ \underline{\underline{C}}^{-1/2} \left(E \underline{\underline{A}} + \lambda^{(1)} \underline{\underline{B}}_1 + \lambda^{(2)} \underline{\underline{B}}_2 + \underline{\underline{B}}\right) \underline{\underline{C}}^{-1/2} + \gamma \right\} \left(\underline{\underline{C}}^{1/2} \underline{\underline{c}}\right) = 0. \tag{129}$$

The feature of V_{12} being positive or negative definite is shared by the important case of $V_{12}\,(|\underline{r}_1 - \underline{r}_2|)$ being a Yukawa interaction.

The SL-method, as most approximate methods in nuclear physics, meets a problem , when the Pauli principle has to be taken into account for the following reasons. Whereas the solutions of the exact Hamiltonian, symmetric in all particles, must necessarily be symmetric or antisymmetric in all particle coordinates, this is in general not the case for a truncated Hamiltonian, like the one we consider here, where the closed shell nucleons are represented by an inert core.

The best one can hope for is then to find a wave function, which gives an extremum for the Hamiltonian in the space of states orthogonal to the occupied core states. This was done in ref.[9] by a method, which is similar to a procedure, suggested in ref.[2].

We add, to the Hamiltonian, a term which is a sum of projection operators on all occupied one- or two-particle states, multiplied by a constant

$$\widetilde{H} = H + T \sum_i |i\rangle\langle i|. \tag{130}$$

If now the constant T becomes very large $\widetilde{H}$ will have eigenfunctions, which are very near to $|i\rangle$, with eigenvalues near to T

$$\widetilde{H}\,|i\rangle \sim T|i\rangle. \tag{131}$$

Other eigenvectors will be orthogonal to these, and in the limit of T going to infinity, these other vectors are the desired extremum states. We shall not here go into details of describing this method, since this was done in ref.[9].

VIII. Numerical examples

The following numerical results are meant only as a brief illustration of some of the points given above. Application of the wave functions to calculation of physics quantities, like cross-sections of transfer reaction are to be found elsewhere.

The first point, which we want to illustrate, is the approximate degeneracy of $\lambda_{n\ell}$ for the spherical Woods-Saxon potential, when n and ℓ form the same oscillator quantum number, $N = 2n + \ell$. For high ℓ values, λ gets smaller, however, in agreement with general expectations. The parameters of the potential are given in table I, and λ's in table II.

The second point is the perturbation admixture of small components, corresponding to $\lambda_{n\ell}$ values far from the dominant ones. As an example, we take the $p_{1/2}$ amplitude, for the state with energy E=-7.215 MeV in ^{186}W. The result of a calculation with a quadrupole deformation as V_{12} are shown in figs. 1,2, which also contain a table of the eigenvalues.

Finally, we show the difference in wave functions found by two diagonalization methods, used in the two-particle case. The truncation of the basis is given by table III, the potential parameters are found in table I, the interaction between the particles

$$V_{12} = \gamma \, e^{-\mu r}/\mu r$$

$$\gamma = -24.1 \text{ MeV} \quad , \mu = 0.21 \, fm^{-1}$$

was found by the proper diagonalization procedure and the same value used in the procedure fo find E.

IX. Concluding remarks

The investigation of the SL method, given here, is not complete. We think here not so much of the mathematical rigour,

where in some cases it is left to the reader to complete the somewhat sketchy proofs. What we have in mind , is the limitations to few-particle problems, to bound states and to non-relativistic problems.

The difficulties of extending the method to the case of many particles are obvious, but so are the difficulties of other methods, and the similarity between the SL basis functions and shell model functions may at least in some cases, together with their completeness properties, give them some advantages compared with oscillator states, plane-waves and other basis functions in use.

The analogous method for unbound states is obviously the Weinberg expansion method, or rather methods, since the ambiguities for positive energies are even larger than here, leading to different possible choices of boundary conditions. The biorthogonality of some of these basis states is a complication. However, with proper generalizations, many of the properties of completeness and convergence are carried over to the positive energies also, see, e.g. /10/. The Weinberg states have been used in nuclear physics, but the above-mentioned features seem not to have thoroughly been exploited, and to do this may be one way of future development. Relativistic problems were not treated here, but, obviously, the Klein-Gordon or Dirac equations may be treated in a similar way as here the Schrödinger equation.

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Table I.

Parameters used in calculating the LS basis, corresponding to tables II and III (I,II), respectively. The spin-orbit force, proportional to $\frac{1}{r}\frac{dV}{dr}\,\underline{\ell}\cdot\underline{s}$, was adjusted in each case to fit the observed spin-orbit splitting.

	R fm	a fm	E MeV
1	$1.36 \cdot (186)^{1/3}$	0.73	-7.215
2	$1.24 \cdot (40)^{1/3}$	0.65	-19.98

Table II.

λ-values for different N and within the oscillator shell N = 6

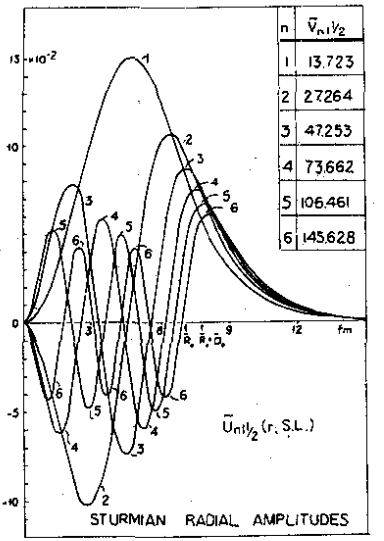
N = 6								N=5	N=7
ℓ,j	0,1/2	2,3/2	2,5/2	4,7/2	4,9/2	6,11/2	6,13/2	1,1/2	5,11/2
λ (Mev)	41.6	42.1	39.9	43.0	37.0	37.6	32.0	33.0	44.4

Table III.

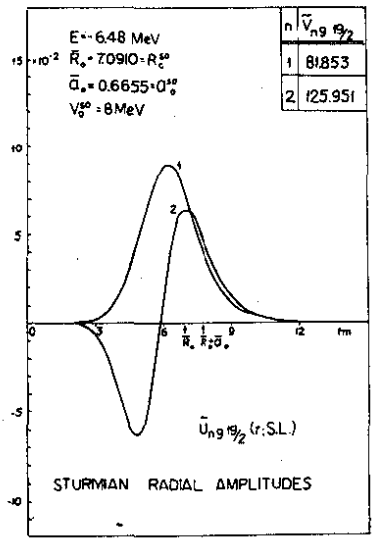
SL coefficients for the two-particle problem, obtained from equation (122) with E as eigenvalue (I) and equation (121) with γ as eigenvalue (II), keeping $E=E_{exp}$. The values of E and E, corresponding to case I are given below the table, as well as the experimental energy E_{exp}, γ =-24.0847

n_1	l_1	j_1	n_2	l_2	j_2	I	II
0	3	7/2	0	3	7/2	0.98438	0.98419
0	3	7/2	1	3	7/2	0.00678	-0.00531
0	3	7/2	2	3	7/2	-0.00716	-0.00506
1	3	7/2	1	3	7/2	0.01609	0.01369
1	3	7/2	2	3	7/2	-0.00138	-0.00263
2	3	7/2	2	3	7/2	0.00415	0.00376
1	1	3/2	1	1	3/2	0.08483	0.09669
1	1	3/2	2	1	3/2	-0.00308	-0.00531
2	1	3/2	2	1	3/2	0.00733	0.00610
0	3	5/2	0	3	5/2	0.09588	0.09206
0	3	5/2	1	3	5/2	-0.00392	-0.00648
1	3	5/2	1	3	5/2	0.00770	0.00746
1	1	1/2	1	1	1/2	0.03604	0.04070
1	1	1/2	2	1	1/2	-0.00199	-0.00336
2	1	1/2	2	1	1/2	0.00407	0.00356
0	4	9/2	0	4	9/2	-0.09575	-0.08874
1	2	5/2	1	2	5/2	-0.02503	-0.02745
2	0	1/2	2	0	1/2	-0.00884	-0.01035
0	4	7/2	0	4	7/2	-0.02954	-0.02899
1	2	3/2	1	2	3/2	-0.01285	-0.01483
0	5	11/2	0	5	11/2	-0.04047	0.03761
0	5	9/2	0	5	9/2	0.01539	0.01504

E_{exp}=-19.84 E=-19.94 E=-19.84



1. Radial wave functions and SL eigenvalues for a $p_{1/2}$ component of ^{182}W, showing components multiplied with the proper c-values, the absolute values being adjusted to the normalization of the total wave function[11].



2. Radial wave functions and SL eigenvalues for a $g_{9/2}$ component of ^{182}W.

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