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

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

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

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 сечений прямых ядерных реакций между сложными ионами. Полнота использованного 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 скорость сходимости полученных рядов не слабее, чем n^{-4}.

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

Different convergence 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 used in nuclear physics.

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

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1. Introduction

Since the Sturm-Liouville expansion method in atomic[1-8] and nuclear [9-18] physics has recently obtained some spreading we find it appropriate here to discuss some of the properties, which make it useful. These are tacitly assumed in other papers, where the main aim is to use it for calculation of principal properties or numerical comparison with other methods whereas a more mathematical demonstration of its convergence properties, etc., has earlier been given only in very general terms[19].

The term Sturm-Liouville problem is used for a wide class of eigenvalue problems of the type

$$-\Delta f_i + \sum_s \lambda_{i,s} V_s f_i = 0, \qquad (1)$$

where f_i satisfy certain boundary conditions, or more specifically for the one-dimensional problem of this type, sometimes even more specifically for the problem in a finite interval.

Even then, the concept is sufficiently general to include, e.g., the one dimensional Schrödinger eigenvalue problem.

In physics, however, the term Sturm-Liouville problem is often used in another restricted sense, as distinct from the Schrödinger eigenvalue problem. The coefficient of an eigenvalue (V_s above) depends on the choice of coordinates. The problem is then called a Sturm-Liouville, in the following abbreviated

to SL, problem in $\lambda_{i,s}$ only when V_s depends on the ordinary "physical" coordinates (or relative coordinates), e.g., like $V(r)$ if spherical coordinates are used. We can, in the one-dimensional case, always bring the LS eigenvalue problem to a form where V_s is 1. However, this means introduction of new, artificial coordinates which in most of our work are an unnecessary complication.

The usefullness of this SL problem in quantum mechanics is closely tied up with some physical facts. With the possible exception of the forces which bind the quarks together to form baryons, it seems that all physical forces are finite in the sense, that the potential between particles goes to a finite limit for large distances between them. This means that the Schrödinger equation which describes the motion of particles interacting with such forces will have a continuous spectrum, as well as possibly a bound spectrum.

Now, the problem is often met that functions which are, e.g., eigenfunctions of a complicated problem, are characterized by their expansion in eigenfunctions of a comparatively simple problem. If this is of the Schrödinger type, the continuum eigenfunctions must in general be included in order that the functions form a complete set for the expansion. It is often more convenient to use an eigenfunction problem with a discrete spectrum, as the Schrödinger equation with a harmonic oscillator or a box potential to provide the expansion base. However, just the unphysical character of these potentials may cause further troubles, as, e.g., bad convergence in some region of the space.

In general, one may say, that when physical problems are solved by expanding some functions in a complete set of functions, it is advantageous if the members of this set or at least some of them are as similar as possible to the functions which are to be expanded, e.g., by satisfying a differential equation of a similar type. In this respect, an SL method, in the meaning of the word given above is frequently advantageous. It will often be possible to find an SL set, which is discrete, and for which

the expansion satisfies certain particularly sharp convergence conditions, as the "uniform convergence of the logarithm", defined below in Section III.

The SL expansion was first introduced in quantum mechanical calculations by Epstein[1], immediately after the publication of Schrödinger's first paper. The aim was to get a simple expansion set for calculation of the Stark effect, and the SL-set was that of solutions to Schrödinger-hydrogen-like equations, with a fixed binding energy and varying charges

$$\left(-\Delta + \frac{2m}{\hbar^2}\left(\frac{z_i e^2}{r} - E\right)\right) f_i = 0. \qquad (2)$$

It is here a great simplification, that the eigenfunctions have simple analytic forms (a polynomial z_i times an exponential function in r). In other ways, this example is rather particular by the potential being singular at the origin and of long range, too.

We are here mainly dealing with the Woods-Saxon potential, which is generally accepted to be a good approximation to the nucleon-nucleus interaction, thus looking at equations of the type

$$\left(-\frac{\hbar^2}{2m}\Delta + V_0 + \lambda_i V - E\right) f_i = 0$$
$$V = -\left(1 + \exp\left(\frac{r-R}{a}\right)\right)^{-1}, \qquad (3)$$

where V_0 may represent, e.g., additional Coulomb terms. The main property of the potential (the factor of λ_i) which has made it convenient for nuclear physics problems, is, that it is of finite range, nearly flat in a certain internal region, and varies mainly in a definite surface region of the order of magnitude a. Another property, which we are going to make use of, is that it is different from 0 everywhere in space. It has no singularities.

II. General mathematical properties of Sturm-Liouville expansions

The general theory of SL expansions was well established for a long time[19]. We shall briefly recapitulate it here, with particular reference to the above-mentioned potentials. Theorems about completeness and convergence can in some cases conveniently be proved directly from the 3-dimensional form, and we will write our equations in a way where the dimensionality is not stated explicitly. It seems, that for many reasons, it is appropriate to go over to integral equations.

Writing our equation (1) as

$$((H_0 - \mathcal{E}) + \lambda_i V) f_i(r) = 0 , \tag{4}$$

where, in the general case, $H_0 = -\frac{\hbar^2}{2m}\Delta + V_0$ we may go over to the integral form

$$sign(V)\,\lambda_i |V|^{1/2} (\mathcal{E} - H_0)^{-1} |V|^{1/2} g_i(r) = g_i(r) , \tag{5}$$

where $g_i(r) \equiv |V(r)|^{1/2} f_i(r)$, and the reciprocal operator $(\mathcal{E}-H_0)^{-1}$ generally must be an integral operator.

We may also write (5) as

$$\lambda_i \int K(r, r') g_i(r')\, dr' = g_i(r) . \tag{6}$$

Here, when H_0 is self-ajoint, K is symmetric. This is fundamental for the proof of the expansion theorem below.

We must obviously have

$$\int g_i^+ g_j\, dr = \int f_i^+ V f_j\, dr = N_i \delta_{ij} , \tag{7}$$

where we can choose the normalisation

$$N_i = -1 . \tag{8}$$

In the case , when $H_0 = -\Delta$ (3-dimensions, neutrons) (here and in many following equations we use $2m = \hbar = 1$) we can explicitly write

$$K(\underline{r}) = sign(v) \int |V(r)|^{1/2} \frac{e^{-\varkappa|\underline{r}-\underline{r}'|}}{|\underline{r}-\underline{r}'|} |V(r')|^{1/2} d\underline{r}', \qquad (9)$$

$$\varkappa^2 = |\varepsilon|.$$

The usual requirement which quantum mechanics puts on our functions and therefore also on the basis is that they belong to the Hilbert space $\mathcal{L}^2$ of square integrable functions (of, say, n variables).

It is clear that in order that the eigenfunction equation would have a meaning, some limitations must be put on K, and the most convenient is that also the kernel of K is square integrable, i.e., belongs to $\mathcal{L}^2$ (of, say, $2n$ variables). For such kernels, the Schwartz' inequality will ensure that when it acts on functions belonging to $\mathcal{L}^2$ it gives again functions belonging to $\mathcal{L}^2$, and that products of such transformations belong to $\mathcal{L}^2$ again. According to the theorems of Hilbert and Schmidt, any function g, belonging to $\mathcal{L}^2$ now admits a development

$$g = h + \sum_i^\infty \frac{c_i}{\lambda_i} g_i, \qquad (10)$$

where $Kh = 0$.

So we may also write

$$d = Kg = \sum_i^\infty c_i g_i. \qquad (11)$$

This expansion is convergent in the mean. Mercer's theorem /20/ states further that if all but a finite number of the eigenvalues of K have the same sign, the convergence of the expansion is uniform and absolute. This means, that if

$$d(\underline{r}) = \sum_{n=0}^\infty c_n g_n(\underline{r}) \qquad (12)$$

and

$$d_N(\underline{r}) = \sum_{n=0}^N c_n g_n(\underline{r}) \qquad (13)$$

then it is possible to find an $N_0(\varepsilon)$ such that

$$\left| d_N(\underline{r}) - d(\underline{r}) \right| \leq \varepsilon \qquad N > N_0(\varepsilon) \cdot \tag{14}$$

From (5) we may also write (11) as

$$\begin{aligned} f &= |V|^{-1/2} d = sign(V)(\mathcal{E} - H_0)^{-1} |V|^{1/2} g \\ &= \sum_{i=0}^{\infty} e_i f_i \end{aligned} \tag{15}$$

so we see, that any f , for which

$$|V|^{1/2} d = sign(V)(\mathcal{E} - H_0)^{-1} V f \in \mathcal{L}^2 \tag{16}$$

has an expansion (12) with the convergence of

$$|V|^{1/2} f_N(\underline{r}) = |V|^{1/2} \sum_{i=0}^{N} c_i f_i \tag{17}$$

being absolute and uniform.

From (15) and (16) we see the necessity of $V \neq 0$ almost everywhere.

Since (16) is fulfilled, when V goes to zero <u>slower</u> than a Gaussian function, for $r \to \infty$ and f is an oscillator eigenfunction, we will, for the potentials considered here, have a set of f's which is complete in $\mathcal{L}^2$ (one or 3-dimensions), so in this sense $\{f_i\}$ is complete in the relevant Hilbert space.

The uniform convergence of (17) is of course not identical to uniform convergence of f_N, but we shall see below, that in some important cases, we can prove an even stronger type of convergence of the f_N's .

To what extent do the potentials used in nuclear and atomic physics satisfy the above requirements?

The property of K being $\mathcal{L}^2$ is satisfied by all nuclear potentials in use, and with slight modifications for large r-values (screening) $r^{-1} \Rightarrow e^{-cr} r^{-1}$

also for the Coulomb potential.

Definiteness, i.e., all λ_i have the same sign - is obtained, e.g., from (9) if V is always positive (negative), so this is the case both for the pure Coulomb case and for V given by (3).

For protons, the total single particle Hamiltonian contains a combination of this attractive potential and a repulsive Coulomb potential. If this combination is used for V, K is not definite. However, due to the long range of the Coulomb potential, it seems more reasonable to use an SL basis where this is kept fixed and included in $H_0(V_0)$.

Since the Coulomb potential is repulsive, we will then only have eigenvalues corresponding to an attractive nuclear potential, i.e., K is again definite.

When spin coordinates are included in the space $\underline{X}$, we can introduce spin-orbit terms in the Hamiltonian. Since these are generally of the type $\frac{1}{r}\frac{dV}{dr}\underline{\ell}\cdot\underline{s}$ they will occur with both signs, and again, if they are included in V, we will lose the definitenesss property. If we include them in H_0, a combination of a repulsive central potential and an attractive spin orbit term could give a state in $\mathcal{L}^2$. However, there will only be a finite number of such states, for each ℓ, corresponding to the finite number of bound states in the pure spin orbit potential. For large values of ℓ such states are again excluded due to the centrifugal barrier.

We will then conclude, that if we use the SL expansion in the ways indicated here, it gives us an absolutely and uniformly convergent expansion in the above meaning of all functions which are in $\mathcal{L}^2$ of the single particle coordinate space (including spin coordinates).

III. Particular convergence properties

Physically significant quantities are in quantum mechanics calculated from the wave functions ψ_i, as matrix elements

$$A_{ij} = \int \psi_i^* A \psi_j \, d\tau, \qquad (18)$$

where A is an operator, in the general case depending on coordinates and derivatives. When the ψ's satisfy a Schrödinger equation, the derivatives can in general be transformed into integral operators. It is now seen, that the property of absolute, uniform convergence is in general sufficient to ensure, that quantities, like A_{ij} calculated by approximate wave functions

$$(A_{ij})_N = \int (\psi_i^*)_N \, A (\psi_j)_N \, d\tau \qquad (19)$$

are also absolutely convergent, and this shows the physical significance of the expansion theorem, in the SL case at least for such operators which converge stronger than $|V|^{1/2}$ for $r \to \infty$. However, the existence of infinitely many systems of SL functions with different potentials, etc., (and in this connection we may use the term for the Schrödinger expansion as well) makes it desirable to find some criteria to distinguish between them.

Of course, one important criterium may be the easiness with which (1) is solved. This depends, however, on the available computers and programs, and we shall concentrate on more mathematical criteria.

The first is the fastness of the convergence, i.e., for a given ε, which method leads to the smallest N_0. At the end of this section, we shall discuss this convergence fastness and see, that in many cases, the SL expansion is superior to other expansion methods.

There is however another problem, which is important when the same nuclear wave functions are tested in many different experiments. The uniform convergence ensures only that the difference for a given matrix element $|(A_{ij})_N - A_{ij}|$ can be made smaller than a given ε for $N > N_0(\varepsilon)$. But in different experiments matrix elements of very different magnitude are investigated. If now we have fixed $N_0(\varepsilon)$, so that a good accuracy is obtained for a given operator A, it is by no means sure, that the same $N_0(\varepsilon)$ gives a good accuracy for another operator, B.

If, e.g., $|B_{ij}| < \varepsilon$, the inequality $|(B_{ij})_N - B_{ij}| < \varepsilon$ is of no use.

Generally speaking, the problem is that certain operators

test small components of the wave function, and it would be desirable if our expansions were good, also for these components. Mathematically speaking, we can say that this is the case, if we have not only

$$|\psi_N(\underline{r}) - \psi(\underline{r})| < f \qquad \text{independent of } (\underline{r}) \tag{20}$$

but also

$$\left|\frac{\psi_N(\underline{r})}{\psi(\underline{r})} - 1\right| < f \qquad \text{independent of } (\underline{r}) \tag{21}$$

$$\text{for almost all } \underline{r} \ (|\underline{r} - \underline{r}_i| > \delta, \psi(\underline{r}_i) = 0)$$

$$\text{for } N > N_0(f).$$

Since "uniform relative convergence" or similar expressions do not give a clear idea of what is meant, we shall instead talk about "uniform convergence of the logarithm". In fact, (21) implies

$$|\ln \psi_N(\underline{r}) - \ln \psi(\underline{r})| < f_1 = |\ln(1-f)| \tag{22}$$

$$\text{independent of } (\underline{r})$$

$$\text{for } N > N_0(f(f_1))$$

and conversely, (22) implies

$$\left|\frac{\psi_N(\underline{r})}{\psi(\underline{r})} - 1\right| < f_2 = |e^{f_1} - 1| \tag{23}$$

$$\text{independent of } (\underline{r})$$

$$\text{for } N > N_0(f_1(f_2)).$$

We shall now find some conditions which ensure the SL expansion to have uniform convergence of the logarithm. We shall for simplicity look at the one dimensional (radial) case only, corresponding to experiments testing regions of different distance $\underline{r}$ from the center of the potential (as, e.g., in heavy ion transfer with different energies).

So we look at the expansion (11), where f satisfies

$$(H_0 + \lambda V + V_1 - E) f = 0 \tag{24}$$

and f_ℓ

$$(H_0 + \lambda_\ell V - \mathcal{E}) f_\ell = 0 \tag{25}$$

with $\mathcal{E} = E$,
where H_0 is in the case of neutrons $-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2}$ and the boundary condition for f and f_ℓ are $f(0) = f_\ell(0) = 0$. Now

$$\frac{f_N(r)}{f(r)} = \frac{f_N(r_0)}{f(r_0)} + \int_{r_0}^{r} dr' \, \frac{W(f_N(r'), f(r'))}{f^2(r')}, \tag{26}$$

where r_0 and r are chosen in such a way, that the integral exists. We shall also express the Wronskian

$$W_N(r') \equiv W(f_N(r'), f(r')) \tag{27}$$

in terms of an integral:

$$W_N(r') - W_N(r_1) = \int_{r_1}^{r'} \left(\frac{d}{dr} W_N(r)\right) dr$$
$$= -\sum_{n=0}^{N} \int_0^\infty f(r) V f_n(r) dr \int_{r_1}^{r'} dr \, f_n(r)((\lambda_n - 1) V(r) - V_1(r)) f(r), \tag{28}$$

where we have used (24) and (25) and put $\lambda = 1$.
Now

$$W_N(0) = W_N(\infty) = 0 \tag{29}$$

and we may conveniently choose $r_1 = 0$, then

$$W_N(r') = -\sum_{n=0}^{N} \left(\int_0^\infty f(r) V_1(r) f_n(r) dr \int_0^{r'} f_n(r) V(r) f(r) dr \right.$$
$$\left. - \int_0^\infty f(r) V(r) f_n(r) dr \int_0^{r'} f_n(r) V_1(r) f(r) dr \right), \tag{30}$$

where we have once more used (24) and (25).

Let us now suppose, that $V(r)$ is almost everywhere continuous and differentiable, and that there exists a constant, C_1, such that

$$|V_1(r)| < |C_1 V(r)| \qquad \text{for all } r. \tag{31}$$

Then we will have an SL expansion of $h = f\frac{V_1}{V}$ with the same uniform convergence properties as that of f :

$$|V(r)|^{1/2}\,|h_N(r) - h(r)| < \varepsilon \quad \text{for all } r \tag{32}$$

$$\text{for } N > N_0(\varepsilon),$$

where

$$h_N(r) = \sum_{n=0}^{N} f_n(r) \int_0^\infty f_n(r')\, V_1(r')\, f(r')\, dr'. \tag{33}$$

So (30) may also be written

$$\begin{aligned} W_N(r') &= -\int_0^{r'} \left(h_N(r)\, V(r) - f_N(r)\, V_1(r) \right) f(r)\, dr \\ &= -\int_{r'}^{\infty} \left(f_N V_1 - h_N V \right) f\, dr. \end{aligned} \tag{34}$$

In view of the uniform convergence of the expansion of f and h we now have

$$|W_N(r')| < \varepsilon \int_0^{r'} \left(|V(r)| + |V_1(r)| \right)^{1/2} |f(r)|\, dr \tag{35}$$

$$\text{for } N > N_0(\varepsilon) \quad \text{independent of } r'.$$

If now a constant C_2 exists, so that

$$r'^{\beta} \int_{r'}^{\infty} dr\, |V(r)|^{1/2}\, |f(r)| < C_2 f^2(r') \tag{36}$$

$$\text{for } r_0 < r' \leq r \text{ and } \beta > 1$$

we obviously have from (26), that

$$\left| \frac{f_N(r)}{f(r)} - \frac{f_N(r_0)}{f(r_0)} \right| < \varepsilon C_3 \tag{37}$$

$$\text{independent of } r.$$

Now, by the uniform convergence of $|V|^{1/2} f_N$, we can always find (r_o, N_o), so that

$$\left| \frac{f_N(r_o)}{f(r_o)} - 1 \right| < \eta \qquad (38)$$

$$\text{for } N > N_o(\eta),$$

where r_o is at a finite distance from any zero of $|V|^{1/2} f$.

We therefore see, that in all open intervals between the zeroes of $|V|^{1/2} f$, we have uniform convergence of the logarithm, provided c_1 and c_2 exist. The requirement, that $|r - r_i| > \delta$ is, for most zero points r_i's, without implications, since no operator will test the wave function in the neighbourhood of an arbitrary zero. Only those, which are given by the boundary conditions (0 and ∞) are of interest, and have $f_N(r) = 0$ also. In practice, the interval which is most interesting is

$$r_{omax} < r < \infty,$$

where r_{omax} is the largest finite zero of f. That such a largest zero exists is easy to prove (see section V).

The exigency, that c_2 exists is now identical to the requirement that

$$\int_r^\infty dr' |V(r')|^{1/2} e^{-\varkappa r'} < c_2 \exp(-\varkappa r) \qquad (39)$$

$$\text{for } r > r_{omax}$$

or, for the potential of (3) $\varkappa a < 1$.
So, for small $\varkappa$ -values, the condition is always fulfilled. This is also the region, where this convergence property is most needed.

What we have here found, are <u>sufficient</u> conditions for the uniform convergence of the logarithm of $f_N(r)$, and a fortiori of $f_N(r)$ itself. Even Mercer's theorem and its foundation come in this cathegory. These conditions are in the most important cases satisfied by nuclear interactions (potentials).

It is not easy to find necessary conditions for V and V_1, either for the uniform convergence of f_N, or for that of the logarithm. This is clear from the fact, that any finite series in the f_n's possesses both convergence properties, and at the same time can be thought of as a solution of (24), in general

defining a V_1 without physical sense, but imposing no new restrictions on V. The importance of the uniform convergence of the logarithm is seen, when we compare the Sturmian expansion with an expansion of f (a solution of (24)) on harmonic oscillator wave functions, which may be uniformly convergent, but where, nevertheless, e.g., if it is an overlap function for particle transfer, calculation of precise cross sections for heavy ion transfer processes will require a larger basis for smaller energies.

Also the question of how fast is the convergence of the SL expansion may be elucidated in the case defined by equations (24) - (25), still keeping $E = \mathcal{E}$. In this expansion we have the coefficient of f

$$C_n = -\int_0^\infty f\, V f_n\, dr = \lambda_n^{-1} \int_0^\infty f\,(H_0 - \mathcal{E}) f_n\, dr =$$

$$= -\lambda_n^{-1} \int_0^\infty f\,(\lambda V + V_1) f_n\, dr = (\lambda - \lambda_n)^{-1} \int_0^\infty f\, V_1 f_n\, dr = \tag{40}$$

$$= -(\lambda - \lambda_n)^{-1} C_n^I .$$

As we shall show below, in Section V, λ_n is roughly proportional to n^2. Since C_n^I is bounded, when V_1 is bounded, as we shall assume, the series will converge rapidly. Looking at the first integral for c_n in (40), this may be said to be due to the more and more rapid oscillations of f_n as n increases. However, the last integral in (40) has the same property. The c_n^I is actually the SL expansion coefficient of

$$h^I = f\,\frac{V_1}{V} = f\,W_1 , \tag{41}$$

which , for the V, V_1 we are interested in, belongs to $\mathcal{L}^2$. Now h^I satisfies the equation

$$(H_0 - \mathcal{E}) h^I = V^I h^I + U^I \frac{d}{dr} h^I$$

$$V^I = \left(\frac{d}{dr} \ln W_1\right)^2 + \frac{d^2}{dr^2} \ln W_1 - V_1 - \lambda V \tag{42}$$

$$U^I = 2\,\frac{d}{dr} \ln W_1 .$$

So

$$c_n^I = -\int h^I V f_n \, dr = \frac{1}{\lambda_n} \int f_n (H_o - \mathcal{E}) h^I dr$$

$$= \frac{1}{\lambda_n} c_n^{II} \,, \tag{43}$$

where c_n^{II} is the coefficient of f_n in the SL expansion of

$$h^{II} = -\frac{1}{V} \left(V^I h^I + U^I \frac{d}{dr} h^I \right). \tag{44}$$

For some potentials, V, and residual terms, V_1, the argumentation leading from f to h^I and from h^I to h^{II} can be repeated over and over. However, already the convergence, faster than λ_n^{-2}, implied by (40)-(44) when h^{II} is bounded, is very fast, and the main problem in practical calculations seems rather to be, for which n values, this type of convergence sets in (see further Section VII). The boundedness of h^{II} is easily proved in the important case where V is of the Woods-Saxon type (3), and V_1 is proportional to its radial derivative. This is the type of radial dependence, met in the 3-dimensional case, when V_1 represents a coupling to an oscillating or static surface deformation, as we shall see in Section VI. The c's will then further contain a vector coupling coefficient, which, however, has no influence on the convergence properties considered here.

IV. The eigenvalue problems of the truncated Sturm-Liouville expansion

Our aim with the SL expansion is to approximate the bound state solutions of the Schrödinger equation for one or more particles, which is an eigenvalue problem. This naturally finds its counterpart, when a truncated expansion is used, in a set of independent linear equations for the coefficients. The requirement, that these equations have a solution, i.e. that their determinant is zero, then determines the eigenvalue.

Now, the Schrödinger equation will in general contain a number of constants, which could be adjusted in order to attain this. Whenever these constants enter the equation in a linear way,

the problem can be solved by standard techniques, as a matrix diagonalization problem. One possibility is the traditional search for E, when the different terms in the potential are given. It should then be remembered, however, that the desirable convergence properties, treated in the last section, obviously depend on the fact that we have put $E = \mathcal{E}$. In order to achieve this, we would therefore have to adjust $\mathcal{E}$, by some sort of iteration . Since the energies are experimentally known, and important features of the wave functions depend directly on these energies, a reasonable alternative would be to change the potential terms in the Hamiltonian in such a way, that $E = \mathcal{E} =$ the expérimental value. This might again be done by iteration , but if there are the linear parameters of the interactions, the coupling constants or potential depths, which are changed, it can also be achieved directly in nearly the same way as E is found. Below in section VII, we shall look closer at this problem in the case of two interacting particles in a potential. First, we shall, however, look at the question of how to obtain sets of linear equations for the coefficients.

Different methods to achieve this have been used in the literature[10,11,17].

They are equivalent in the limit of $N \to \infty$, but not for finite N, and it is therefore of interest to compare them. We shall do so only for a simplified example, which, however, reveals the main features of the general problem.

We look again at the Schrödinger equation

$$(H - E) f = 0. \tag{45}$$

It is obviously equivalent to

$$U(H - E) f = 0 , \tag{46}$$

where U is an arbitrary function, which is different from zero everywhere in configuration space. We can now multiply (46) by the members of a complete set of functions $\{f_j'\}$ and integrate, thus obtaining

$$\sum_i c_i \int f_j'^{*} U (H - E) f_i \, d\tau = \sum_i M_{ji} c_i = 0 . \tag{47}$$

Then the eigenvalue problem is

$$\mathcal{D}et\,(M_{ji}) = 0. \tag{48}$$

This has meaning, if we truncate in such a way as to get the same number of independent functions f_i and f_i'.

We are interested only in the case, that the f_j''s are again SL-functions. Then two choices of U are useful: U=V and U = 1.

The first gives

$$\sum_i c_i \left(\int f_j^* V H f_i \, d\tau + E \delta_{ij} \right) = 0 \tag{49}$$

corresponding to the **diagonalization** of the matrix VH, which is not Hermitian, but nevertheless must have at least some real eigenvalues.

We shall specialize to

$$H = -\Delta + \lambda V + \gamma V_1 \;, \quad E = \varepsilon \;, \tag{50}$$

where the constants λ and γ are introduced to show the linear dependence on potential depth, etc., explicitly.

Now we get with $U = 1$

$$\sum_i c_i \left(-\gamma \int f_j^* V_1 f_i \, d\tau + (\lambda - \lambda_i) \delta_{ij} \right) = 0 \tag{51}$$

this is a Hermitian eigenvelue problem with λ as an eigenvalue (and can be transformed into one with γ as an eigenvalue). We shall now concentrate on the one-dimensional (radial) case, the same as in section III, but with the further simplification that

$$\begin{array}{lll} \text{for} & 0 \le r < R & V = -1, \; V_1 = 0 \\ - & R \le r < S & V = -\tau, \; V_1 = -1 \\ - & S \le r < \infty & V = 0, \; V_1 = 0 \;. \end{array} \tag{52}$$

We introduce the names

$$\int_R^S f_j^* f_i \, dr = \sigma_{ji} \;, \quad \int_0^R f_j^* f_i \, dr = V_{ji} \tag{53}$$

from which we see

$$V_{ji} + \tau \sigma_{ji} = \delta_{ji} \tag{54}$$

for $E = \mathcal{E}$ we now have in the two cases with U=V and U=1 respectively

$$\sum_i^N c_i' ((\lambda' - \lambda_i)(V_{ij} + \tau^2 \sigma_{ij}) + \tau \gamma \sigma_{ij}) = 0 \tag{55}$$

and

$$\sum_i^N c_i ((\lambda - \lambda_i)\delta_{ij} - \gamma \sigma_{ij}) = 0 . \tag{56}$$

In order to understand the effect of the truncation, we shall now introduce a 1. order perturbation approach for the solution of (56), valid when the $|\gamma \sigma_{ij}|$ are sufficiently small compared to any $|\lambda_\ell - \lambda_\kappa|$. If a truncation will be useful at all, such a perturbation expansion must converge fast for sufficiently high i and/or j.

$$\begin{aligned} c_0 &= 1 \qquad \text{(definition)} \\ c_i\ (i \neq 0) &= -\frac{\gamma \sigma_{i0}}{\lambda_i - \lambda_0} \\ \lambda &= \lambda_0 - \gamma \sigma_{00} . \end{aligned} \tag{57}$$

Due to the non-diagonal terms containing λ_i , (55) does not immediately lend itself to a perturbation approach. However, since (55) and (56) are equivalent for large N, we shall try to solve (55) with the ansatz

$$\begin{aligned} c_0' &= 1 \\ c_i'\ (i \neq 0) &= c_i + d_i \\ \lambda' &= \lambda + \mu , \end{aligned} \tag{58}$$

where μ and d_i are considered to be small. To their determination we then have, neglecting terms of the order $d_i \mu$, $d_i \gamma \delta \mu$ and γ^2 , the equation

$$\gamma\left(\sigma_{j0}+\sum_{i\neq 0}^{N}\sigma_{ji}\,\sigma_{i0}\,(\tau^{2}-\tau)-\tau\,\sigma_{0j}\right.$$

$$\left.+\,\sigma_{00}\,\sigma_{j0}\,(\tau^{2}-\tau)\right)+d_{j}\,(\lambda_{0}-\lambda_{j}) \qquad (59)$$

$$+\mu\left(\sigma_{j0}\,(\tau^{2}-\tau)+\delta_{j0}\right)+\sum_{i\neq 0}^{N}d_{i}\,(\tau^{2}-\tau)\,(\lambda_{0}-\lambda_{i})\,\sigma_{ij}=0.$$

Now the completeness relation

$$\sum_{i=0}^{\infty}g_{i}(r')\,g_{i}(r)=\delta(r'-r) \qquad (60)$$

for the function

$$V_{1}(r)=-V_{1}^{2}(r) \qquad (61)$$

gives

$$\int_{0}^{\infty}f_{j}\,V_{1}\,f_{0}\,dr=\int_{0}^{\infty}dr\,f_{j}(r)\,V_{1}(r)\,|V(r)|\sum_{i=0}^{\infty}f_{i}(r)\int_{0}^{\infty}f_{i}(r')\,V_{1}\,|V(r')|^{1/2}\,f_{0}(r')\,dr' \qquad (62)$$

or

$$\sigma_{j0}=\tau\sum_{i=0}^{\infty}\sigma_{ji}\,\sigma_{i0}\ . \qquad (63)$$

This series is, according to what was proved earlier, absolutely convergent.

With no truncation, we have $d_{i}=\mu=0$, and, which is easily proved, no other solution.

In the truncated case we have

$$d_{j}\,(\lambda_{0}-\lambda_{j})+\sum_{i\neq 0}^{N}d_{i}\,(\tau^{2}-\tau)\,(\lambda_{0}-\lambda_{i})\,\sigma_{ij}$$

$$+\mu\left(\delta_{0j}+\sigma_{0j}\,(\tau^{2}-\tau)\right)=-\gamma\sum_{i>N}^{\infty}\sigma_{ji}\,(\tau^{2}-\tau)\,\sigma_{i0} \qquad (64)$$

which is N + 1 equations to determine the N + 1 unknowns $d_{j}\,(j=1\ldots N),\mu$.

Introducing

$$X_{i}\,(i\neq 0)\equiv d_{i}\,(\lambda_{0}-\lambda_{i}) \qquad (65)$$

$$X_0 \equiv \mu , \quad Y_j \equiv \sum_{i>N}^{\infty} \sigma_{ji} \sigma_{i0}$$

we get

$$X_i = \gamma (\tau - \tau^2) \sum_{j=0}^{N} (A^{-1})_{ij} Y_j , \tag{66}$$

where

$$A_{ij} \equiv \delta_{ij} + (\tau^2 - \tau)\sigma_{ij} = \int f_i V^2 f_j \, d\tau . \tag{67}$$

Since the potential V is meant to give a rough picture of a nuclear potential, we shall assume, that the "surface part" of it, $V=-\tau$ for $R \leq r \leq S$ is small, but not <u>very</u> small compared to the "volume part", V = -1 for $0 \leq r \leq R$, and that

$$\alpha \leq \tau < 1 , \tag{68}$$

where α is a positive number, (say, $0.25 \leq \alpha \leq 0.5$).

Then, an order of magnitude estimate for $X_i(N)$ is obtained from (66), replacing A_{ij} with δ_{ij} , i.e.,

$$X_i \approx \gamma (\tau - \tau^2) \sum_{j>N} \sigma_{ij} \sigma_{j0} \tag{69}$$

for the estimate of $Y_i(N)$ we shall further assume, that N is so large, that all $f_i \ (i>N)$ are well approximated by sine functions for $R \leq r \leq S$. Then, with the proper normalization of the f's , we have

$$|Y_i| < c_i \sum_{j>N} \frac{1}{j(j-i)} < C \frac{i}{N} , \tag{70}$$

where c_i and C are at most of an order of magnitude of unity.

It is seen, that the effect of truncation is somewhat similar to a renormalisation of γ by the factor $1 + \frac{C}{N}(\tau \pm \tau)$ when going from one method to the other.

The factor V gives a spatial truncation. For $\tau = 1$, the two methods are equivalent, but not for $\tau = 0$, since the completeness relation, leading to (63) is not valid any more. However, the lack of completeness invalidates both approaches. This is

clear also from the fact, that for $\tau = 0$, all f_i' and therefore also $f' = \sum c_i f_i'$ (independent of the truncation) satisfy

$$(H_0 - E) f' = 0 \quad , \quad r > R \tag{71}$$

but f should satisfy

$$(H_0 - \delta - E) f = 0 \quad , \quad \delta > r > R \tag{72}$$

so it is necessarily different from f'. Obviously in order to get near to f, if δ is large, it is an advantage to have a large τ -value. It is seen from (41),etc.,also, that the convergence of the SL expansion for small τ values is slowed down by the factor $V_1/V = \delta/\tau$ which enters into h^{τ},etc. One could think of using a base with V different from that of the total Hamiltonian. But if V_1 is small or has cancelling contributions, this would slow down the convergence. The equivalent idea, with realistic nuclear potentials would be to use a basis with a large value of R or a. However, for reasons similar to those given above, this is of limited help.

The question which of the two methods yields the most correct result, is not clearly stated. We must instead choose an operator, $\hat{\theta}$, and ask, which method gives the expectation value $\langle \psi | \hat{\theta} | \psi \rangle$ nearest to the correct one $\langle \psi_0 | \hat{\theta} | \psi_0 \rangle$. The best choice would presumably be $\hat{\theta} = |\psi_0\rangle\langle\psi_0|$, but since we do not know $|\psi_0\rangle$ we must instead choose an operator which is minimized by $|\psi_0\rangle$. Now, the eigenvalue problem (51) of determining $\lambda = \lambda_\nu$ with the basis $\{ f_i', i \leq N \}$ is equivalent to the minimization of H-E in the same basis, with the subsidiary condition that the solution

$$\psi = \sum_{i \leq N} c_i f_i \tag{73}$$

is normalized by the SL-normalization

$$\int \psi^* (H - E) \psi \, d\tau = \min \quad , \quad \int |\psi|^2 V \, d\tau = -1. \tag{74}$$

If we only look at the lowest value of $\lambda(N)$ corresponding to $\psi_0(N)$ (ground state) the minimum is an absolute one and by an appropriate choice of H, all cases can be reduced to this. Since the states $\psi_\nu(N)$ form a complete basis in the space $\{f_i, i \leq N\}$ with the same orthonormality as the f's, the mean value of H-E (74) can also be written

$$\int \psi^*(H-E)\psi d\tau = \sum_{\nu \leq N} |e_\nu|^2 (\lambda_\nu - \lambda). \qquad (75)$$

which is obviously minimized by $c_\nu = \delta_{\nu\nu_0}$.

So, when N goes to infinity, $\lambda_0(N)$ goes to λ and the mean value is roughly proportional to the square of the deviation of ψ from the exact solution ψ_0 .

Therefore, when the deviations are sufficiently small, the function which gives the smallest mean value in (74) is the best approximation. But since, as we have just stated, (51) is, for the limited basis $\{f_i, i \leq N\}$, equivalent to the minimization problem of this same space, (51) must be the "best" solution which can be constructed from the functions $\{f_i, i \leq N\}$. Just how good it is, can be inferred from the general convergence properties of the SL expansion, which grant that the neglected sum $\sum_{i>N} c_i^2 \lambda_i$, will go to zero faster than some negative power $(\lambda_N)^{-p}$.

It should be noted, that these arguments are valid only for sufficiently high N-values. No guarantee exists, that for some small value of N, (51) is actually better than (49). Note also, that (49), or the equivalent eigenvalue problem for the energy, is not equivalent to a variational principle, because of its non-Hermiticity.

Another argument, in favour of the diagonalization with $u = 1$, is, that in perturbation theory, where ψ is expanded in powers of λ , the 1. order terms are given by (57), independent of the truncation, whereas we have just shown, that this is not the case for $u = V$.

Conclusion

We have here considered some problems of convergence of the Sturm-Liouville expansion technique, with particular regard to nuclear problems, where the natural basis is the one, where the SL functions satisfy Schrödinger-like equations with a fixed energy but different depths of a potential well of the Woods-Saxon shape.

The properties of this potential, which are essential for our discussion (essentially negative definiteness of the potential and finiteness of certain integrals of it) are obviously shared by the two other potentials of common use in nuclear physics, particularly in few-body problems, the Yukawa and the Hulthen potentials.

For reasons of simplicity, the discussion was mainly dealing with one-dimensional problems, most of the features proved are, however, with due modifications, found in the more interesting multi-dimensional cases, too.

The convergence properties (16,17) of the expansion mean, that in any finite region of configuration space, every function which is continuous almost everywhere can be approximated arbitrarily well by the SL-series.

For a class of functions, satisfying a Schrödinger equation with a potential which decreases with increasing r not slower than that of the base, we showed that in the most interesting case of not too strongly bound particles, the SL-expansion has the property of uniform convergence of the logarithm (21) in the important region of $r \to \infty$, and we also showed, that the terms in the expansion go to zero not slower than n^{-4}.

We looked at the eigenvalue problem, and found a relation between different types of diagonalization proposed in the literature; the Hermitian methods (56) were shown to possess some advantages as compared to others.

In a forthcoming paper, we shall discuss some remaining question: the shape of the Sturmian functions, the special problems of the three-dimensional expansion, as well as of the six-dimensional one, used for 2 particle problems, and some applications to concrete problems of nuclear physics.

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