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SEMIANALYTICAL METHOD FOR TREATMENT OF THE N-BODY PROBLEM WITH COMPLEX TOTAL ENERGY WITHIN THE HYPERHARMONICS APPROACH

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1 Introduction

This work has two aims. The first one is to display the main points of the method which we develop considering the problem of N neutral particles with the complex total energy close to zero. The second aim is to attract attention to the problem of long-range interactions always emerging in the standard hyperharmonics approach (**HHA**).

To begin with, we recall some well-known facts.

In the **HHA** [1] the wave-function Ψ of the considered N-body state is represented as the scalar product

$$\Psi(r,\Omega,\mathrm{p}) = r^{2-3N/2}(Yu) \equiv r^{2-3N/2} \sum_{[L]=[L_{\min}]}^{[L_{\max}]} Y_{[L]}(\Omega) u_{[L]}(r,\mathrm{p}) \tag{1}$$

of the row Y of the suitable hyperharmonics and the column u of the searched hyperradial components.

The problem for u reads as the following matrix equation

$$[(\partial_r^2 + p^2)I + Dr^{-2} - V(r)]u(r,\mathrm{p}) = 0 \tag{2a}$$

supplemented with the regular boundary condition at the origin,

$$u(r,\mathrm{p}) \to 0, \quad r \to 0, \tag{2b}$$

and an appropriate boundary condition at infinity

$$u(r,\mathrm{p}) \to U(r,\mathrm{p}), \quad r \to \infty. \tag{2c}$$

Here p is the total hypermomentum, $p^2 = E$ is the total energy, I and D are the diagonal matrices defined by

$$I \equiv diag(1), \quad D \equiv diag(\lambda(\lambda+1)), \quad \lambda \equiv L + 3(N-2)/2,$$

and the potential matrix V has the elements

$$V_{[L][L']} \equiv < Y_{[L]}| \sum_{i<j} V_{ij} |Y_{[L']} >, \tag{3}$$

and finally, U is assumed to be the known column–function and is chosen so that the wave-function (1) describes the physical process of interest.

As is well–known, the **HHA** has an essential peculiarity. The point is that, in general, all the potential matrix elements decrease at infinity too slowly [1],

$$V_{[L][L']}(r) \to r^{-m}, \quad r \to \infty, \quad m \geq 3, \tag{4}$$

even when the two–body potentials denoted in eqs.(3) by V_{ij} are the short–range ones.

This long–range behaviour of the potential matrix elements causes serious difficulties for the direct numerical solution of the problem (2) in the low–energy region. The matter is that when the total energy goes to zero, the contribution to calculated observables generated by the long–range potential tails becomes dominant. The detailed explanation and series of the numerical illustrations of this statement can be found in works [2] and [3]. So, working within the **HHA** in the low–energy region one indispensably has to solve the essential problem: how to take correctly into account the long–range asymptotics (4) of the potential matrix elements when the total energy is complex and close to zero?

There are two cases (the N-body bound–state problem and the problem of the so-called democratic N-body resonances) when we have found a way to answer this question.

2 Method

In essence, only two main ideas form the basis of our method. The first idea is to reduce the original problem (2) to a simpler differential problem convenient both for the numerical solution and for analytical investigation. The second idea is to solve the new problem numerically in the inner region $0 \leq r \leq d < \infty$ with a high accuracy and then to construct the solution of this problem in the outer region $r > d$ analytically. In this way we treat the problem exactly, where the potential matrix has a complicated r-dependence, and use simple inverse–power functions to approximate the potential matrix elements at large enough r, where eqs.(4) are valid.

In the following we assume that the asymptotics U of (2c) is known and all the two–body potentials are uniformly converging series

$$V_{ij}(x_{ij}) = \sum_{n=-1}^{\infty} V_{ijn} x_{ij}^n \quad as \quad x_{ij} \to 0 \tag{5a}$$

and are functions modulo–integrable on the semi-axis $0 \leq x_{ij} \leq \infty$,

$$|V_{ij}(x_{ij})| \,|\in \mathbf{L}^1_{[0,\infty]}. \tag{5b}$$

Note that in view of the standard potential scattering theory [4] these conditions are general enough.

To reformulate the original problem (2), we perform a series of simple constructions which are well–known in the general theory of ordinary differential equations [5].

We start with introduction of the fundamental matrix $\Phi = |\Phi_{[L],[L']}|$ of the regular solutions and define each its column $\Phi^{[L']}$ ($[L'] = [L_{\min}], \ldots, [L_{\max}]$) as the solution of eq.(2a), i.e. the equation

$$[(\partial_r^2 + p^2)I + Dr^{-2} - V(r)]\Phi^{[L']}(r,p) = 0, \tag{6a}$$

with the special asymptotic behaviour

$$\Phi_{[L]}^{[L']}(r,p) \equiv \Phi_{[L][L']} \to r^{\lambda'+1}(\delta_{[L],[L']} + O(r^{2-m})(1 - \delta_{[L][L']})), \quad r \to 0, \tag{6b}$$

established by Palumbo in Ref.[6] for arbitrary N-body systems with two–body interactions satisfying the relations (5a). As he has shown, the number m in eqs.(6b) stands for the power of the leading term ($O(r^{-m})$) of the potential matrix asymptotics as $r \to 0$.

Since the column–functions $\Phi^{[L']}$ have different asymptotics at the origin and obey the same eq.(6a), they are linearly–independent and their complete set forms the fundamental system [5,6] of regular solutions of the initial eq.(2a) under the condition (2b).

Hence, once this system is build, we can represent the particular (physical) solution u as a linear combination

$$u(r, \mathbf{p}) = (\Phi(r, p) A(\mathbf{p})) \tag{7}$$

of all the fundamental solutions with numerical coefficients $A_{[L']}$ which we can choose so as a way to satisfy the boundary condition (2c) describing the asymptotics of u at infinity. Thus, we have the following asymptotic relation

$$(\Phi(r, p) A(\mathbf{p})) \rightarrow U(r, \mathbf{p}), \quad r \rightarrow \infty, \tag{8}$$

defining the column A of the numerical coefficients. As we explain in the following, it is very convenient to apply to the problem (6) the variable–constant method [5] known in quantum mechanics as a linear version of the variable–phase approach [7]. Using these methods we look for the matrix Φ as a bilinear form

$$\Phi(r, p) = (1/2)((h^{(+)}(x) f^{(+)}(r, p)) + (h^{(-)}(x) f^{(-)}(r, p))) \tag{9}$$

in which $x \equiv pr$, $\quad h^{(\pm)} \equiv diag(h_\lambda^{(\pm)})$ are diagonal matrices containing the Rikkati–Hankel functions [8] and $f^{(\pm)} = |f^{(\pm)}_{[L],[L']}|$ are the so-called amplitude matrix–functions obeying (by definition) the matrix Lagrange identity [5]

$$(\partial_r f^{(+)} h^{(+)}) + (\partial_r f^{(-)} h^{(-)}) \equiv 0. \tag{10}$$

With the usual trick based on the substitution of Φ in the form (9) into the problem (6) and using identity (10) and the Wronskian relation for the Rikkaty–Hankel functions we arrive at the problem defining the amplitude functions. It reads as

$$\partial_r f^{(\pm)} = (\pm i/2p) h^{(\mp)} V((h^{(+)} f^{(+)}) + (h^{(-)} f^{(-)})) \tag{11a}$$

$$f^{(\pm)} \rightarrow I, \quad 0 < r < r_0 \rightarrow 0. \tag{11b}$$

Thus, we have reformulated the initial problem (2) in terms of the amplitude functions. They obey linear, homogeneous and first–order ordinary differential problem. Evidently, the problem like this is very simple for numerical solution and for analytical investigations. Hence, the first idea of the method is totally accomplished.

Now we have deal with the amplitude functions and our next problem is how to construct them.

To this end we realize the second idea of the method as follows. Introducing a division parameter d we divide the semi-axis $\mathbf{R}^+$ of the hyperradius r into the internal $(r \leq d)$ and external $(r > d)$ regions. We assume that the division parameter d is large enough so that the inequality $\mid p \mid d \gg 1$ holds and moreover, in the external region the potential matrix is the uniformly converging series

$$V(r) = \sum_{n\geq 3}^{\infty} V_n r^{-n} \tag{12}$$

containing the numerical matrices V_n .

In the internal region we calculate the amplitude functions numerically. Note that here the potential matrix is usually a very complicated function of r and therefore in this region it is impossible to find the amplitude functions explicitly. However, according to the theory of ordinary differential equations [5], under conditions (5) the problem for these functions has a unique and finite solution on any finite interval, for example, when $0 < r \leq d$. Therefore, there are no special difficulties for high–accuracy numerical solution of this problem in the internal region. For these reasons we suggest to find the amplitude functions in this region numerically. When they are calculated, we shift the boundary conditions for eqs.(11a) to the left boundary of the external region, i.e. to the point d, and then we treat the obtained differential problem in the external region analytically. It seems to be reasonable because in this region (i.e., when $\mid x \mid > \mid p \mid d \gg 1$) the potential matrix has the simple asymptotic representation (12), the Rikkati–Hankel functions can be expanded in simple series [8],

$$h_\lambda^{(\pm)}(x) = \exp(\pm ix) S_\lambda^{(\pm)}(x), \tag{13a}$$

$$S^{(\pm)}(x) \equiv \sigma_\lambda^{(\pm)} \sum_{m=0}^{\infty} (\lambda + 1/2, m)(\mp 2ix)^{(-m)}, \tag{13b}$$

$$\sigma_\lambda^{(\pm)} \equiv \exp(\mp i\pi(\lambda+1)/2) \tag{13c}$$

and, moreover, as we show in the following, the amplitude functions, in general, infinitely increase or rapidly oscillate at infinity. Therefore, they cannot be evaluated numerically at a large hyperradius.

By using the expansions (12) and (13) we have found the asymptotic representations for the amplitude functions in the external region. Unfortunately, in this letter we are compelled to omit all the details. Therefore, we present only our final result. It means that in the external region the amplitude functions are sums

$$f^{(\pm)}(x) = Z_1^{(\pm)}(p,x) + \exp(\mp 2ix) Z_2^{(\pm)}(p,x) \tag{14a}$$

containing the **smooth** and **finite** matrix–functions representable as asymptotical series

$$Z_i^{(\pm)}(p,x) = x^{k(i-1)} \sum_{n=0}^{\infty} C_{in}^{(\pm)}(p) x^{-n}, \quad i = 1, 2, \tag{14b}$$

in which the numerical matrices $C_{in}^{(\pm)}$ are well-defined by the linear and recursive (over index n) matrix–equations and k stands for the power of leading term ($O(r^{-k})$) in the expansion (12).

By the proof of formulae (14) we have realized the second idea of our method and go to discussion of most interesting results we have obtained within this method.

3 Results

The first result can be formulated as follows. Due to the long–range asymptotics (12) of the potential matrix, the amplitude functions have essential singularities at $r = \infty$. Indeed, owing to eqs.(14), $f^{(+)}$and $f^{(-)}$ diverge exponentially if $Jmp > 0$ and $Jmp < 0$, respectively. On the other hand, by iterating eqs.(11a) written in the integral form one can show that $f^{(\pm)}$ have finite limits as $r \to \infty$, if all the elements of V decrease at infinity more rapidly than any $\exp(-\mu r)$ with an arbitrary $\mu > 0$; for example, if the potential matrix is cut-off at some point b, i.e. if it is put that $V \equiv 0$ for all $r \geq b$. In this case, owing to eqs.(11a), we have $f^{(\pm)}(r,p) \equiv f^{(\pm)}(b,p)$ for any $r \geq b$. Hence, when we employ the cut-off procedure (and thus neglect the long–range tail of V), we actually replace the correct asymptotics (14a) of $f^{(\pm)}$ by quite different asymptotics, namely by the constants $f^{(\pm)}(b,p)$.

What are the corollaries of this replacement?

The second result is actually the answer to this question. In the following, to simplify the explanation, we restrict ourselves to the minimal approximation of **HHA**. In this approximation $[L] = [L'] = [L_{\min}], \lambda = \lambda_{\min}$, by definition, and therefore, all the matrices are one-dimensional and all the formulae are essentially simplified. For example, there are only two amplitude functions and a single hyperradial component which, by virtue of eqs.(7-9), reads as

$$u = u_{[L_{\min}]} = A\Phi = (A/2)(h_\lambda^{(+)} f^{(+)} + h_\lambda^{(-)} f^{(-)}) \tag{15}$$

Let the potential matrix be cut at a certain point $b > d$. Then, using eqs.(11),(13) and (15) we can write the asymptotics of u as

$$u \to A(\exp(ix)\sigma_\lambda^{(-)} f^{(+)}(b,p) + \exp(-ix)\sigma_\lambda^{(+)} f^{(-)}(b,p))/2, \quad r \to \infty. \tag{16}$$

Now let us assume that the hypermomentum p is such that

$$f^{(-)}(b,p) = 0. \tag{17}$$

Then the asymptotics (16) becomes simpler,

$$u \to A exp(ix)\sigma_\lambda^{(-)} f^{(+)}(b,p)/2, \quad r \to \infty, \tag{18}$$

and there is a trivial correspondence between the position of p on the complex p-plane and the kind of behaviour of u at a large hyperradius. Indeed, owing to (18), u has the bound-state asymptotics $(\exp(- \mid p \mid r))$ if $p{=}iJmp$ and $Jmp > 0$, u has the virtual-state asymptotics $(\exp(+ \mid p \mid r))$, if $p{=}iJmp$ and $Jmp < 0$, and finally, the asymptotics of u reads like resonance–state asymptotics $(exp(iRepr+ \mid Jmp \mid r))$ when $Rep > 0$ and $Jmp < 0$.

It is interesting to remark that, due to the representations (15) and (16) and the above–mentioned correspondence, the function $f^{(-)}(b,p)$ is an analog of the two–body Jost function [4].

We would like to emphasize an essential fact. We have specially used the variable phase approach to get the key–equations, i.e. eqs.(11), giving us a brilliant possibility to analyze the contribution from the tail of the potential matrix to all the functions we have dealt with and, moreover, to introduce some very useful functions having an apparent physical meaning and making this analysis to be extremely clearest.

For example, we mention about two very useful complex functions $P(b)$ and $E(b)$. They have an apparent physical meaning and are defined in the spirit of the variable phase approach as follows. Clearly, the solution p of eq.(17) depends on the value of b. We denote by $P(b)$ the function describing this dependence and then we let $E(b) \equiv P^2(b)$. The function $P(b)$ shows how the solution p of eq.(17) moves on the complex p-plane when the cut-off parameter b changes. The function $E(b)$ describes the trajectory of the squared solution of this equation on the complex–energy plane. By this definition, the values $P(\infty)$ and $E(\infty)$ correspond to the non-cut-off potential matrix and, for instance, the difference $E(\infty) - E(b)$ is the absolute contribution from the potential tail to the total energy.

Now we would like to discuss the behaviuor of the functions $P(b)$ and $E(b)$ for a three–neutron system in the P^-- doublet state. Applying our method we have investigated these functions in the case when the neutron–neutron singlet potential is the square–well and is of the depth -13.4Mev and width 2.65fm.

As we have established, 1) when the potential matrix is non-cut-off, the 3n-system has no bound or democratic–resonances states, which confirms the conclusion that is common for all earlier treatments [9] of this system, 2) however, when the potential matrix is cut-off at an arbitrary point $b < \infty$, there is an infinite series of democratic 3n-resonances.

How have we found those resonances?

First, we have calculated the trajectories $P(b)$ and $E(b)$ of one resonance for some finite values of b and then using the asymptotics (14) we have interpolated $P(b)$ and $E(b)$ to the point $b = \infty$. To represent these trajectories, it seems to be sufficient to present only four their points. They correspond to the following values of the cut-off parameter $b(fm) = 100, 400, 6000, \infty$ and they are such that $100P(b)(fm^{-1}) = (4 - i3), (1 - i1), (0.05, -i0.05), (0, i0)$ and $E(b)(Kev) = (10, -i6), (-0.2, -i5), (-0.01, -i0.03), (0., i0)$, respectively.

We specially recall these points to show how one makes the physically incorrect conclusion when one neglects a very weak but a long–range potential tail. So let us artificially cut-off the effective interaction at a finite point, say, at $b = 6000 fm$. Then we readily conclude that a 3n-system has a resonance state with a non-zero energy $E = E(6000) = -(10, i30)Ev$. Clearly, this conclusion is incorrect because taking account of the residual long–range tail of this interaction (in the considered example from 6000 (fm) up to $\infty(fm)$) we get a quite different result $E = E(\infty) = (0, i0)$ meaning that there is no physical resonance.

The above–mentioned example is also very illuminative in the following aspects. It demonstrates that the contribution from the long–range tail of interaction to the calculated energy of the resonance–state is dominant. Moreover, this example shows that the low–energy three–neutron resonance–states exist only when the interaction is **artificially** cut-off. Therefore, such resonances which are in essence unphysical and are generated by the cut-off procedure will be called as *artificial* resonances.

Before to go further, we point out an interesting fact. As it is known [10], in the two-body systems with a short–range interaction there are the so-called false resonances which immediately disappear when the interaction is cut-off. By our definition, artificial resonances are of quite a different nature: they exist when the effective interaction is cut-off and disappear when this interaction is totally switched on.

As a next stage of our treatment of the three–neutron P-state, we have set $b = 1000 fm$ and found 17 resonances numerically. Their positions on the complex p-plane is described with good accuracy as follows. The first resonance has $p = (0.001, i0.005) fm^{-1}$. All the resonances locate on the straight line given by the equation $Jmp = -0.05(Rep + 0.1)$ and the distance between any neighboring resonances is about $0.0015 fm^{-1}$ being measured along this line.

And finally, we have analytically proved that all these resonances belong to the infinite series of artificial resonances whose trajectories are aproximately defined by two coupled equations

$$(bJmP)^3(3(ReP/JmP)^2 - 1) \doteq exp(-2bJmP)sin(2bReP), \tag{19a}$$

$$3JmP/ReP = tan(2bReP), \tag{19b}$$

we have derived from eq.(17) using formulae (14b) and (16b). Due to the periodical property of the tangent function, eqs.(19) have an infinite series of solutions. When $b \to \infty$, the distances between the neighboring solutions go to zero, all the solutions condense into straight line coinciding with the real semi-axis of the p-plane. In other words, with growing the cut-off parameter b all resonances move to the real positive axis of the complex p-plane, in the limit $b = \infty$ all of them reach this axis and transform into the non-resonance scattering states.

As we hope, we have apparently demonstrated that working within the **HHA** one has always to analyze the cut-off procedure and correctly take into account the long–range tail of the potential matrix.

The third result is the explanation how the latter can be done within our method. By using the representations (13-16) we write the asymptotics of u in the following form

$$u \to (A/2)(F^{(+)}(x)\exp(ix) + F^{(-)}(x)\exp(-ix)), \quad r \to \infty, \tag{20a}$$

where

$$F^{(\pm)} \equiv S^{(\pm)} Z_1^{(\pm)} + S^{(\mp)} Z_2^{(\mp)} \qquad (20b)$$

are *smooth* and *finite* functions in contrast with the amplitude functions.

Now let us assume that p is such that

$$F^{(-)}(pr) \to 0 \quad as \quad r \to \infty. \qquad (21)$$

Then formula (20a) is reduced to

$$u \to (A/2) F^{(+)}(x) \exp(ix) \qquad (22)$$

and we can again establish the correspondence between the kind of asymptotics behaviuor of u and the position of p on the complex p-plane. Evidently, this correspondence is the same as mentioned above.

Now we cut-off the potential matrix at a certain point $b > d$. Then, owing to eqs.(11a) and (20b) the functions $f^{(\pm)}$ and $F^{(\pm)}$ do not change at $r \geq b$, in particular, the equality $F^{(-)}(pr) = F^{(-)}(pb)$ is valid for all $r \geq b$, and therefore, the limit relation (21) is transformed into the following equation $F^{(-)}(pb) = 0$. Since $F^{(-)}$ is a smooth and finite function, each solution of this equation approximates the corresponding solution of the initial relation (21) with a high accuracy if b is large enough but finite. This guarantees us against unphysical conclusions.

The fourth result is very important for the standard potential scattering theory. In this theory, the Jost function of the two-body problem is defined as a limit of $f^{(-)}(r,p)$ when $r \to \infty$. As it is emphasised in all textbooks (see, for instance, Ref. [4]), this limit does not exist for long-range potentials. The expression (14a) displays the difficulty: $f^{(-)}$ diverges exponentially if $Jmp < 0$. To overcome this problem, we suggest 1) to define $F^{(-)}$ of (20b) as the Jost solution of the two-body problem, 2) to introduce the corresponding Jost function as $F^{(-)}$ taken at the point $r = \infty$, and 3) to use both these functions in practice.

4 Conclusion

As we have shown, in the low-energy region the long-range tail of the potential matrix plays an essential role and for this reason one has to take this tail into account, which can be made by our method expounded in this work.

References

[1] *Fabre de la Ripelle, M.:* Ann. Phys. **147**, 281 (1982)

[2] *Bosveld, G.D. and Schellingerhout, N.V.:* Report 231, Groningen: University of Groningen, 1989

[3] *Pupyshev, V.V. and Solovtsova, O.P.:* IJMP. **A7**, 2713 (1992)

[4] *Taylor, J.R.:* Scattering Theory. New York, London, Sydney, Toronto: John Wiley & Sons, 1972.

[5] *Hille, E.:* Ordinary Differential Equations in the Complex Domain. New York: Wiley-Interscience, 1976.

[6] *Palumbo, F.:* Phys. Lett. **B69**, 275 (1977)

[7] *Calogero, F.:* Variable Phase Approach to Potential Scattering. New York: Acad. Press, 1967.

[8] *Abramowitz, M. and Stegun, I.A.:* Handbook of Mathematical Functions. Washington: D.C., 1972.

[9] *Möller, K. and Orlov, Yu.V.:* Particles and Nuclei **20**, 1341 (1989)

[10] *Bas', A.I., Zel'dovich, Ya.B., Perelomov A.M.:* Scattering, Reactions and Disintegrations in Non-Relativitic Quantum Mechanics. Moscow: Nauka, 1971 (in Russian).

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