ON THE SOLUTION OF THE SCHRÖDINGER EQUATION THROUGH CONTINUED FRACTIONS

J. A. Mignaco

Centro Brasileiro de Pesquisas Físicas (CNPq), Rio de Janeiro, Brasil

ABSTRACT - The domain of interest for the applications of a method to solve the Schrödinger equation through continued fractions is studied. It is argued that the method applies almost equally well to quantum mechanical regimes (lower energy levels, low energy scattering) as well as to semiclassical ones simultaneously; this is illustrated by the example of the central power law potentials $r^{\nu}(\nu>0)$. The explanation of this behaviour is given in terms of the mathematical approximations involved and its relationship to physically interesting quantities.

MAY / 79

I. INTRODUCTION

A method aimed to solve second order ordinary linear differential equation through continued fractions[1] has been applied recently to obtain exact[2] and approximate[3] solutions of the Schrödinger equation for central potentials. Bound states and scattering are considered and solved in a very similar footing with this method. A number of exact results (some new) were got for bound states and a good approximation is obtained since the start in other cases. For scattering, as usual, it was harder to obtain good results than for bound states, but results compare well with other procedures. There is to our knowledge no analytic results concerning the expected domain of application of this method in most physical cases considered. This is the situation also regarding the convergence of the solution in general. Known theorems[2] [3] of convergence are not applicable in many cases.

The motivation for the present article is to provide some hints on the properties of the systems where the solutions are seen to converge heuristically. Since continued fractions are not yet a very familiar object for physicists, we think that it is useful to illustrate or exemplify how they work or in which sense do they provide a sensible approximation for central potentials.

As we shall exhibit below at first sight continued fractions for the Schrödinger equation seem to provide and exact or a quite approximate solution in two non overlapping domains at one time. One is the extreme quantum mechanical physical domain, embracing ground state levels and first excited ones for bound states and the very low energy scattering, where

wave mechanical properties are important. The other is the semiclassical domain of higher energy levels with large quantum numbers, or of scattering with large impact parameters. We shall discuss below how we can understand this feature from the mathematical approximation involved since we shall show that it coresponds precisely to these two different physical cases. To be more specific, an order of approximation in the continued fraction corresponds to neglecting higher derivatives of the Schrödinger wave function, and we then obtain a better approximation (or even an exact solution) whenever these higher derivatives in the required solution are small (or zero); this is precisely the case for the lower bound states, for slow colliding particles and for states with large angular momentum(*).

The text is organized as follows. In section II we recall in a sketchy way the fundamentals of the method used by Refs.(2) and (3). A short account of the results it presented for the applications already made, specially referring to our own previous work(3). Section III covers a rough quantitative study of the domain of application for the potential r^{ν}, providing a concrete sample of the method. Finally, the end section IV is devoted to an analysis of the preceding ones and to advance a possible interpretation that allows to understand them in rather precise terms.

(*) A transformation of the radial coordinate translates this argument to the new variable in all cases where this transformation appears advisable to simplify the problem at hand.

II. THE METHOD AND ITS APPLICATIONS

We shall just give the fundamentals of the method, for more details the reader may refer to Refs. (1), (2) and (3).

Let us take to start the differential equation

$$y = B_{01} \frac{dy}{dx} + B_{02} \frac{d^2y}{dx^2} \tag{1}$$

with B_{0i} (i=1,2) functions of the dependent variable and of a set of parameters fixed by the physical problem (for instance, energy, angular momentum, coupling constants, potential ranges, etc.). Deriving successively we obtain a system of three terms relations

$$y^{(n)} = B_{n,n+1}\, y^{(n+1)} + B_{n,n+2}\, y^{(n+2)} \quad , \quad n=1,2,... \tag{2}$$

with

$$y^{(j)} = \frac{d^j y}{dx^j}$$

and the B_{jk} (k=j+1, j+2) are functions made out of B_{0i}(i=1,2) and of its derivatives up to order j. Substituting each time

$$\frac{y^{(n)}}{y^{(n+1)}} = B_{n,n+1} + B_{n,n+2} \frac{1}{\left(\frac{y^{(n+1)}}{y^{(n+2)}}\right)}$$

we obtain a continued fraction:

$$\frac{y}{y'} = B_{01} + \cfrac{B_{02}}{B_{12} + \cfrac{B_{13}}{B_{23} + \ldots}} \qquad (3)$$

An approximant of order n (n= 1, 2,...) is obtained by definition putting $B_{n,n+2} = 0$ or $\left(\frac{y^{(n+2)}}{y^{(n+1)}}\right) = 0$, and is of the form

$$\left(\frac{y}{y'}\right)_n = \frac{S_{0n}}{S_{1n}} \qquad n= 1, 2, \ldots \qquad (4)$$

where S_{ij} is a (tridiagonal) determinant found by Perron[1] and Mignaco and Miraglia[3b] satisfying

$$S_{ik} = B_{i,i+1}\, S_{i+1,k} + B_{i,i+2}\, S_{i+2,k} \qquad (5)$$

with $S_{i,i} = 1$, $S_{i,i+1} = B_{i,i+1}$, $S_{ij} = 0$ $(j < i)$.

In this or in a slightly modified version this method was applied to a number of potentials in the radial Shrö - dinger equation

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \left(k^2 - \frac{\ell(\ell+1)}{r^2} - U(r)\right)\right] R_{k\ell}(r) = 0 \qquad (6)$$

$$k^2 = \frac{2mE}{\hbar^2} \quad , \quad U(r) = \frac{2m\,V(r)}{\hbar^2}$$

or to differential equations obtained starting from it.

Table I summarizes the relevant information, and in the next section we consider another simple application.

In brief, the outstanding features of the method as emerging from the analyses made in Refs. (2) and specially (3) are the following:

For bound states:

a) The lower order approximants reproduce or give a better approximation for the lower energy levels.

b) For the potentials r^2 and r^{-1} the energy levels with large principal quantum number are exactly given by the lower approximants.

For scattering states:

a) For given angular momentum, the lower order approximants provide a better description the lower is the energy.

b) For given energy in the intermediate energy range, the lower order approximants give a better descrption as the angular momentum is higher.

Both cases a) refer to solutions where the quantum mechanical characteristics of the system are the more important ones. On the other hand, cases b) refer to semi-classical situations where JWKB approximations work satisfactorily.

It is amusing that continued fractions work well in both cases. Since no physical assumption is made to

obtain an approximant it is the mathematics of the game that will explain this feature. This we shall analyze after considering the example of the next section to furnish a stronger support.

III. THE POTENTIAL r^{ν} ($\nu>0$)

Let us consider in Eq.(6)

$$V(r) = g^2 r^{\nu} \qquad \nu > 0 \qquad (7)$$

$$U(r) = \gamma^2 r^{\nu} \qquad (7')$$

If we examine the behaviour of the radial equation (6) and subtract the dominant contributions at the singular points r=0 and r=∞ , the general solution is of the form

$$R_{k\ell}(r) = r^{\ell} \exp\left(- \frac{2\gamma}{\nu + 2} r^{\frac{\nu+2}{2}} \right) \cdot v_{k\ell}(r) \qquad (8)$$

where $v_{k\ell}(r)$ is of course regular in both points. Notice that we are not allowed to extrapolate (8) to $\nu < 0$. We shall now consider two different equations; one results from the substitution of (8) into (6), and is:

$$\left\{ \frac{d^2}{dr^2} - 2\left[\gamma r^{\frac{\nu}{2}} - (\ell+1) r^{-1} \right] \frac{d}{dr} + \left[k^2 - \{ 2(\ell+1) + \frac{\nu}{2} \} \gamma r^{\frac{\nu-2}{2}} \right] \right\} v_{k\ell}(r) = 0 \qquad (9)$$

and the other from the subsequent change of variable

$$z = \gamma r^{\frac{\nu+2}{2}} \qquad (10)$$

and is

$$\left\{ z\frac{d^2}{dz^2} + \frac{1}{\nu+2}\left[\nu + 4(\ell+1) - 4z\right]\frac{d}{dz} + \frac{4}{(\nu+2)^2}\left[k^2\gamma^{-\frac{4}{\nu+2}} z^{\frac{2-\nu}{\nu+2}} - \right.\right.$$

$$\left.\left. - 2(\ell+1) - \frac{\nu}{2}\right]\right\} v_{k\ell}(z) = 0 \qquad (11)$$

In the following, we shall consider just the n=1 approximants since we are willing to settle a rough quanti - tative behaviour(*). Searching for the lowest eigenvalue we must look at the solutions of (9) and (11) such that they don't have any node, as is done in Ref. (3a). We arrive to a couple of relations between the energy of levels with no nodes in this approximation and the coupling. They are

$$k^2 = \gamma^{\frac{4}{\nu+2}}\left[2(\ell+1) + \frac{\nu}{2}\right](\ell+1)^{\frac{\nu-2}{\nu+2}} \qquad (12)$$

coming from Eq. (9) and

$$k^2 = \gamma^{\frac{4}{\nu+2}}\left[2(\ell+1) + \frac{\nu}{2}\right]\left(\ell + 1 + \frac{\nu}{4}\right)^{\frac{\nu-2}{\nu+2}} \qquad (13)$$

obtained from Eq.(11). The dependence on would just result from dimensional analysis, and the ground state corresponds to setting $\ell=0$. How do Eqs. (12) and (13) compare with the true answer ?

In general an exact or even a numerical result, is not available for all ν and then we shall compare with other approximate expressions as well.

(*) This potential is currently being studied in detail with Marcia L. Ramos.

The first approximate expression is obtained using a poor man's version of the Heisenberg principle currently used in courses on Quantum Mechanics. Starting with

$$E = \frac{p^2}{2m} + g^2 r^\nu$$

and putting

$$p = \frac{\hbar}{r}$$

and then minimizing E, obtains

$$k^2 = \gamma^{\frac{4}{\nu+2}} \left(\frac{\nu}{2}\right)^{\frac{2}{\nu+2}} \left(1 + \frac{\nu}{2}\right) \qquad (14)$$

Another set of approximate values comes out from the more sophisticated functional version of the uncertainty principle due to Sobolev and used by Lieb[4] in his work on the stability of matter. It provides an absolute lower bound for the energy of a system and in our case we obtain:

$$k^2 = \gamma^{\frac{4}{\nu+2}} \left[2^{-3}\, 3^{3/2}\, \pi^{1/2} (\nu+2) \frac{\Gamma\left(\frac{3}{2}(\nu+2)\right)}{\Gamma\left(\frac{3}{\nu}\right)} \right]^{\frac{2}{3}\frac{\nu}{\nu+2}} \qquad (15)$$

where $\Gamma(x)$ is Euler's Gamma function.

In Table II we have the results of all these appproximations and some exact values for the lower ν values. We notice that for this range of values continued fractions provide a reasonable set of results[7] as was said before for other cases.

Let us now go on to consider another limiting situation in the region of larger quantum numbers. Here comparisons are poor , since there are in general no accurate numbers available .

For continued fractions, in the case of harmonic oscillator and Coulomb potentials, a linear relation existing between the principal quantum numbers and the angular momentum allows to establish the value of higher energy levels just setting ℓ large. We don't know whether a similar relation exists for other potentials, nonetheless it is in general true that higher ℓ values correspond to higher excitations.
We then shall examine our expressions (12) and (13) from this point of view.

On the other hand, we shall translate into the radial equation the known results[8] available for $|x|^{\nu}$ potentials in one dimension, as corresponding to s-waves.

We then compare

$$\alpha_1 = k^2 \, \ell^{-\frac{2}{\nu+2}} \, \gamma^{-\frac{4}{\nu+2}} \simeq 2 \ , \ (\nu<\infty \ , \ \ell >> 1) \qquad (16)$$

and the one dimensional result

$$\alpha_2 = k^2 \gamma^{-\frac{4}{\nu+2}} \ n^{-\frac{2\nu}{\nu+2}} \cong \left[\frac{\pi^{1/2} \ \nu \ \Gamma\left(\frac{3}{2} \ \ \frac{\nu+2}{\nu}\right)}{\Gamma\left(\frac{1}{\nu}\right)} \right]^{\frac{2\nu}{\nu+2}} \qquad (17)$$

$(n >> 1, \nu\text{:even})$

for which we obtain

$\nu = 2$	$\alpha_2 = 2.000$
$\nu = 4$	$\alpha_2 = 2.185$
$\nu = \infty$	$\alpha_2 = 2.467$

Two points are to be mentioned. The first concerns the rather good numerical agreement. The second regards the similarity in the dependence of Eq. (16) on ℓ and of Eq. (17) on n, suggesting a linear relation between the two, at last.

We think that the comparison made is reasonable, though a more refined analysis is desirable, and it again shows the ability of continued fractions to give a reasonable answer in the semiclassical domain.

IV. PROPOSAL, DISCUSSION AND COMMENTS

Our task is now to advance a convincing argument to explain the characteristics of the behaviour of continued fractions. As said before, the explanation should lie in the mathematical approximations involved.

An approximant of order n is obtained neglecting radial derivatives of order higher than n+2. If the solution of our problem would not depend on derivatives higher than the n+1-th, we should arrive at an exact solution. This is the case for all known exact solutions found.

Now, radial derivatives are related to powers of the radial component of the linear momentum operator:

$$p_r = - i \hbar \left(\frac{\partial}{\partial r} + \frac{1}{r} \right) \tag{18}$$

It appears then quite natural that since the lower energy levels have the lower values for p_r, they are candidates to be well represented (approximately) by the lower approximations to the continued fraction.

In the quasi classical limit we have to apply another line of reasoning . S-states involve classically the passage of the particle through the center of force. We should not expect then to represent well low angular momentum states with higher energies. Instead, trajectories having sufficiently large angular momentum are available having a large contribution to energy but with small values on the average, of the radial component of the linear momentum. It is then plausible that these states will be well approximated by lower order approximants .

We then propose that continued fractions solution of the radial Shrödinger equation approximates better the states containing lower average values of the radial component of the linear momentum.

We have two other examples of the applicability of this criterium. The S-levels of the Yukawa potential have a depth that increases with the coupling constant faster than linearly. Since the average energy depends explicitly on the coupling γ^2 in a linear way(*), we may conclude that kinetic energy, as the coupling increases, does not follow the increase in the negative potential energy. We should then expect that, as the coupling increases, a better approximation is obtained from an approximant of fixed order. This is the case, precisely, as illustrated by Fig. 1 of Ref. (3a).

Let us come back to the power law radial potential dealt with in Section III. Applying the virial theorem we get for the rate of the average values of the kinetic and potential energy contributions:

$$\frac{< T >}{< V >} = \frac{\nu}{2}$$

We should then expect to obtain better approximations for lower values of ν, as it was shown in Table II.

For scattering processes a similar line of thought applies. It is evident that at lower energies (larger wave - lenghts) we should obtain better approximations. By the same considerations about the semiclassical range in bound states,

---

(*) An implicit dependence at the average values on γ^2 is surely possible.

it is to be expected that large angular momentum states become well represented by the lower approximants in the intermediate energy region.

To conclude, we think that our analysis provides a clue to carry on applications of continued fractions in the way considered above, at least for central potentials of a simple shape. It would be better, of course, if we would be able to provide a sound analytical foundation of the features discussed. Nonetheless we think that our contribution clears up some aspects of the applications performed and allow for a more intuitive understanding of these mathematical tools.

TABLE I

A summary of the application of continued fractions to the radial Schrödinger equation. $g^2 > 0$, $\mu > 0$ in the expressions below.

POTENTIAL	PARTIAL WAVES	REFERENCE	TYPE OF RESULTS
1. Bound States			
$\frac{1}{2} m\omega^2 r^2$	All	2; 3a	Exact
$- g^2 r^{-1}$	All	2; 3a	Exact
$- g^2 r^{-1} \exp(-\mu r)$	S,P	3a	Approximate
$- g^2 \exp(-\mu r)$	S	2	Exact
$-g^2 \exp(-\mu r)(1-\exp(-\mu r))^{-1}$	S	2	Exact
2. Scattering Only approximate results are obtained			
$-g^2 (\cosh \mu r)^{-2}$	S	2	
$-g^2 \exp(\mu r)$	S	2	
$\pm g^2 r^{-2}$	$\ell \leq 3$	3b	
$\pm g^2 r^{-1} \exp(-\mu r)$	$\ell \leq 10$	3b	

TABLE II

Comparison of exact and approximate values for the ground state energy of the potential r^{ν} ($\nu>0$) with the result of continued fractions

ν	Eq.(12)	Eq.(13)	Eq.(14)	Eq.(15)	Exact
1	2.5000	2.3208	0.9449	1.9478	2.338[5]
2	3.0000	3.0000	2.0000	2.1822	3.000
3	3.5000	3.9145	2.9402	2.2569	
4	4.0000	5.0397	3.7798	2.2798	3.7939[6]
∞	ν	ν^2	ν	2.1079	9.8696

The case $\nu=\infty$ is the infinite potential well of radius 1.

REFERENCES AND NOTES

1) Perron, O., "Die Lehre von den Kettenbrüchen", Mathematischen Wissenschaften, Band 36 (1913)
Ince, E.L., "Ordinary differential equations", Dover Publ.Inc., New York (1956)

2) Biswas, S.N. and Vidhani, T., Journal of Physics A6, 468(1973). We thank professor A. Vaidya, UFRJ, for acquainting us with this important work.

3) a) Garibotti, C.R. and Mignaco, J.A., Zeitschrift für physik A 274, 33 (1975)
b) Mignaco, J.A. and Miraglia, J.E., Zeitschrift für Physik A 280, 1 (1977)

4) Lieb, E.H., Rev. of Mod. Phys. 48, 553 (1976)

5) Flügge, S., "Practical Quantum Mechanics", Springer Verlag (1971), page 101, problem 40.

6) Hioe, F.T. and Montroll, E.W., J. of Math. Phys. 16, 1945 (1975)

7) In connection with Table II let us raise a point. It is seen that Sobolev's - Lieb method results always in smaller energies than any exact result. On the other hand, any state constructed with the help of the solutions of the differential equation would have an energy equal or larger than the ground state

energy. The question is: what kind of vectors are the other states intervening in the (Hilbert) space of Sobolev - Lieb construction ? Classical systems allow for lower energies than quantum ones.

8) Gol'dman, I.I. and Krivchenkov, V.D., "Problems in Quantum Mechanics", Perganon Press and Addison - Wesley Co, Inc. (1961), pages 5 and 64, problem 1-22.