

# Bound states of central fields with wave functions of elementary form

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**ABSTRACT.** We present an easy way (accessible to any beginning student) of generating nontrivial central potentials of such a sort that, for an arbitrary  $l$ -wave, the exact eigenfunctions of the pertinent radial equation can be analytically expressed in terms of elementary functions. No special functions need to be invoked.

**RESUMEN.** En este artículo presentamos una manera simple de generar potenciales centrales no triviales, de tal manera que, para cada valor del momento angular orbital  $l$ , la autofunción solución de la correspondiente ecuación radial puede ser expresada analíticamente en términos de funciones simples. El método es accesible a cualquier estudiante de un curso introductorio de física cuántica, puesto que no se necesitan funciones especiales para la construcción de la función de onda.

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## 1. INTRODUCTION

Situations in which Schrödinger's radial equation can be exactly solved without recourse to special functions are of great pedagogical interest, since the number of such instances that are easily accessible to beginning students is very small indeed.

The radial equation can be analytically solved in closed form, for all values of the angular momentum quantum number  $l$ , in a restricted set of cases (essentially the square-well, the Coulomb potential and the harmonic oscillator) [1]. Nevertheless, there are several families of potentials for which one can express in closed form the  $l = 0$  wave functions in terms of different confluent hypergeometric series. This is the case of the Eckart potentials [2], which with an appropriate choice of parameters yield the celebrated Hulthén potential [3]. We can also mention the Hylleraas, the exponential and the Morse potentials, that are also derived from the Eckart ones. These potentials have been used mostly in connection with molecular physics [4].

Exactly solvable models constitute an invaluable tool in helping to develop quantum intuition and are often useful in gaining deeper understanding into the workings of the quantum world, as vividly illustrated by the recent work of Zakhariiev *et al.* [5-8]. New exactly solvable models have made it possible to formulate a unified quantum picture in which both the direct and the inverse quantum problems are treated on an equal

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footing [5–8]. (Going from the interaction potential to the system's properties constitutes, of course, the direct problem, while going from certain specified properties the system is to possess to the potential needed to that effect poses the inverse problem).

In what follows we shall focus our attention upon the inverse problem. As our aim is that of helping the beginning student to develop quantum intuition, we shall demand that, for an arbitrary  $l$ -wave, the exact eigenfunction be of a very simple functional form. Moreover, as it is desirable for beginners without mathematical sophistication to avoid invoking special functions, we shall look for radial equations such that their eigensolutions be expressed just in terms of elementary functions.

In the *one dimensional* case, a *new*, infinite family of potentials of the polynomial form has been recently shown to possess ground state wave functions of simple analytical form [9] and it should be of pedagogical interest to find a radial analogue. As stated, this is our goal here.

We shall show below how to construct central potentials of such nature that, for a given, *arbitrary*  $l$ -wave, the pertinent eigenfunctions can be expressed in closed form in terms of powers, polynomials and exponentials. In this sense, the present effort goes way beyond the one of Ref. [9], where no methodology is given that may enable the student to determine by himself potentials of the desired properties.

## 2. THE PRESENT METHOD

Using standard notation and atomic units ( $\hbar = m = 1$ ), the radial equation for the reduced wave function  $u_{nl}(r)$  acquires the appearance

$$\frac{d^2 u_{nl}}{dr^2} + 2 \left[ E_{nl} - V(r) - \frac{l(l+1)}{2r^2} \right] u_{nl} = 0, \quad (1)$$

where, for bound states,  $u_{nl}$  usually behaves like  $r^{l+1}$  near the origin and should decay in exponential fashion at infinity. Of course, normalization requires

$$\int_0^\infty dr |u_{nl}(r)|^2 = 1. \quad (2)$$

We shall restrict ourselves to central potentials of the form

$$V(r) = \sum_{k=-1}^N a_k r^k, \quad (3)$$

( $a_k$  real) such that

$$\lim_{r \rightarrow 0} r^2 V(r) = 0, \quad (4)$$

which guarantees the  $r^{l+1}$  behaviour in the neighbourhood of the origin [see Eq. (1)]. Notice that the expression (3) includes as particular cases the Coulomb potential and the harmonic oscillator well. We advance the ansatz

$$u_{nl}(r) = r^{l+1} P_M(r) \exp \left[ -\frac{1}{2} \lambda_0 - \frac{1}{2} \sum_{i=1}^n \lambda_i r^i \right], \tag{5}$$

with  $P_M(r)$  and  $M$ -th degree polynomial that guarantees the correct number of nodes.  $\lambda_0$  is a normalization constant and  $\lambda_1, \dots, \lambda_n$  are real numbers to be determined in terms of the potential-function coefficients  $a_k$ . In addition, one must require  $\lambda_n$  to be positive. It is easy to verify that the above mentioned boundary conditions are satisfied. There is a clear reason for the particular choice of the form (5): it can be justified on Information Theory grounds as the wave function that maximizes the so-called relative entropy [10, 11].

After introduction of (3) and (5) into (1) one realizes that determining the radial wave function (wf) is essentially a matter of choosing the  $\lambda_i$  and the coefficients of  $P_M$  in such a way that corresponding powers of the radial coordinate match on both sides of the radial equation. This is a straightforward but tedious task. However, it constitutes a useful exercise, as techniques which give students practice in performing manipulations leading to special solutions of Schrödinger's equation should always be welcome.

If one adopts such a program, the first conclusion to be reached is that the number of  $\lambda$ 's to be used is given by the potential-function degree as

$$1 + \frac{N}{2} \leq n < 2 + \frac{N}{2}. \tag{6}$$

The second (also an interesting exercise) is to investigate the validity of the method for the Coulomb and the harmonic oscillator potentials. Both cases can be easily tackled with it and one recovers the exact spectrum and analytical wf's. However, it is here convenient to abandon the general discussion, which would become too abstract to be pedagogically useful, and focus our attention upon some concrete situations.

For example, for a nodeless wf ( $P_M = 1$ ), which constitutes the simplest case, one finds, in general, the following expressions relating the coefficients of the potential to those of the wave function:

For  $1 \leq k \leq n - 2$ ,  $k = \text{even}$ ,

$$a_k = \frac{1}{8} \left( \frac{k+2}{2} \right)^2 \lambda_{\frac{k+2}{2}}^2 + \frac{1}{4} \sum_{j=1}^{k/2} j(k+2-j) \lambda_j \lambda_{k+2-j} - \frac{1}{4} (k+2l+3)(k+2) \lambda_{k+2};$$

for  $1 \leq k \leq n - 2$ ,  $k = \text{odd}$ ,

$$a_k = \frac{1}{4} \sum_{j=1}^{\frac{k+1}{2}} j(k+2-j) \lambda_j \lambda_{k+2-j} - \frac{1}{4} (k+2l+3)(k+2) \lambda_{k+2};$$

for  $n - 1 \leq k \leq 2n - 3$ ,  $k = \text{even}$ ,

$$a_k = \frac{1}{8} \left( \frac{k+2}{2} \right)^2 \lambda_{\frac{k+2}{2}}^2 + \frac{1}{4} \sum_{j=k+2-n}^{k/2} j(k+2-j)\lambda_j\lambda_{k+2-j};$$

for  $n - 1 \leq k \leq 2n - 3$ ,  $k = \text{odd}$ ,

$$a_k = \frac{1}{4} \sum_{j=k+2-n}^{\frac{k+1}{2}} j(k+2-j)\lambda_j\lambda_{k+2-j}, \tag{7}$$

which are to be supplemented with

$$a_{-1} = -\frac{l+1}{2}\lambda_1, \quad a_0 = E + \frac{1}{8}\lambda_1^2 - \frac{2l+3}{2}\lambda_2 \tag{8}$$

( $E$  is the pertinent energy eigenvalue), and

$$a_{2n-2} = \frac{1}{8}n^2\lambda_n^2.$$

After an appropriate inversion process, one finds the  $\lambda_i$ 's in terms of the  $a_k$ . One will immediately realize, however, that the  $a_k$  *cannot be chosen arbitrarily*. They must fulfill certain relations among themselves that can be referred to as posing "solvability conditions" for the central field. Only those potentials (3) that comply with these "solvability conditions" lead to reduced radial wave functions of the type that we are interested in here.

### 3. NUMERICAL APPLICATIONS

To be specific, let us consider potentials of the type, say,

$$V(r) = a_2r^2 + a_3r^3 + a_5r^5 + a_8r^8, \tag{10}$$

with  $a_8 > 0$  (any other polynomial in  $r$  is to be treated in similar fashion). We immediately find [*cf.* Eqs. (7)–(9)], the set of relations:

$$\begin{aligned} a_8 &= \frac{25}{8}\lambda_5^2, & a_7 &= 5\lambda_4\lambda_5 = 0, \\ a_6 &= 2\lambda_4^2 + \frac{15}{4}\lambda_3\lambda_5 = 0, & a_5 &= 3\lambda_3\lambda_4 + \frac{5}{2}\lambda_2\lambda_5, \\ a_4 &= \frac{9}{8}\lambda_3^2 + 2\lambda_2\lambda_4 + \frac{5}{4}\lambda_1\lambda_5 = 0, & a_3 &= \frac{3}{2}\lambda_2\lambda_3 + \lambda_1\lambda_4 - \frac{5(l+3)}{2}\lambda_5, \\ a_2 &= \frac{1}{2}\lambda_2^2 + \frac{3}{4}\lambda_1\lambda_3 - (2l+5)\lambda_4, & a_1 &= \frac{1}{2}\lambda_1\lambda_2 - \frac{3(l+2)}{2}\lambda_3 = 0, \\ a_0 &= E + \frac{1}{8}\lambda_1^2 - \frac{2l+3}{2}\lambda_2 = 0, & a_{-1} &= -\frac{l+1}{2}\lambda_1 = 0, \end{aligned} \tag{11}$$

so that

$$\begin{aligned}\lambda_5 &= \frac{2}{5}\sqrt{2a_8}, \\ \lambda_2 &= \frac{a_5}{\sqrt{2a_8}}, \\ \lambda_1 &= \lambda_3 = \lambda_4 = 0, \\ E &= \frac{2l+3}{2} \frac{a_5}{\sqrt{2a_8}}.\end{aligned}\tag{12}$$

In the concomitant process it becomes clear that

$$\begin{aligned}a_3 &= -(l+3)\sqrt{2a_8}, \\ a_2 &= \frac{a_5^2}{4a_8},\end{aligned}\tag{13}$$

the “solvability conditions” in the present instance. Only  $a_5$  and  $a_8$  can be freely chosen, but this is enough to provide one with an infinite family of radial potentials with nodeless eigenstates that can be expressed just in terms of elementary functions. Of course, as the “solvability conditions” involve  $l$ , for a given potential only *one* nodeless wf will be exactly solved in the fashion that interests us here.

The solid curve of Fig. 1 represents the particular instance of (10) for which  $a_5 = -1$  and  $a_8 = 2$  (leading to, for  $l = 2$ ,  $a_3 = -10$  and  $a_2 = 1/8$ ). The dot-dashed line depicts the concomitant, effective potential (including the centrifugal barrier for  $l = 2$ ). The normalized  $1d$ -reduced radial wf for a particle moving in such an effective potential is portrayed in the same figure (dashed line). The position of the corresponding energy level is also indicated.

As a second example consider now the potential function

$$V(r) = a_1r + a_2r^2 + a_3r^3 + a_4r^4 + a_5r^5 + a_8r^8,\tag{14}$$

with  $a_5 = -1$  and  $a_8 = 2$ , with a view to study its associated one-node-states. The polynomial  $P_M$  [cf. Eq. (5)] adopts the simple form  $P_M = r - R$ . The pertinent matching procedure will not only yield the energy eigenvalue and the  $\lambda_i$ 's of the wf but also the position  $R$  of the node.

Here our “solvability conditions” read

$$\begin{aligned}a_1 &= -\frac{a_5}{\sqrt{2a_8}R} - \sqrt{2a_8}R^2, \\ a_2 &= -\frac{a_5^2}{4a_8} - \sqrt{2a_8}R, \\ a_3 &= -(l+4)\sqrt{2a_8}, \\ a_4 &= -\frac{\sqrt{2a_8}}{R},\end{aligned}\tag{15}$$

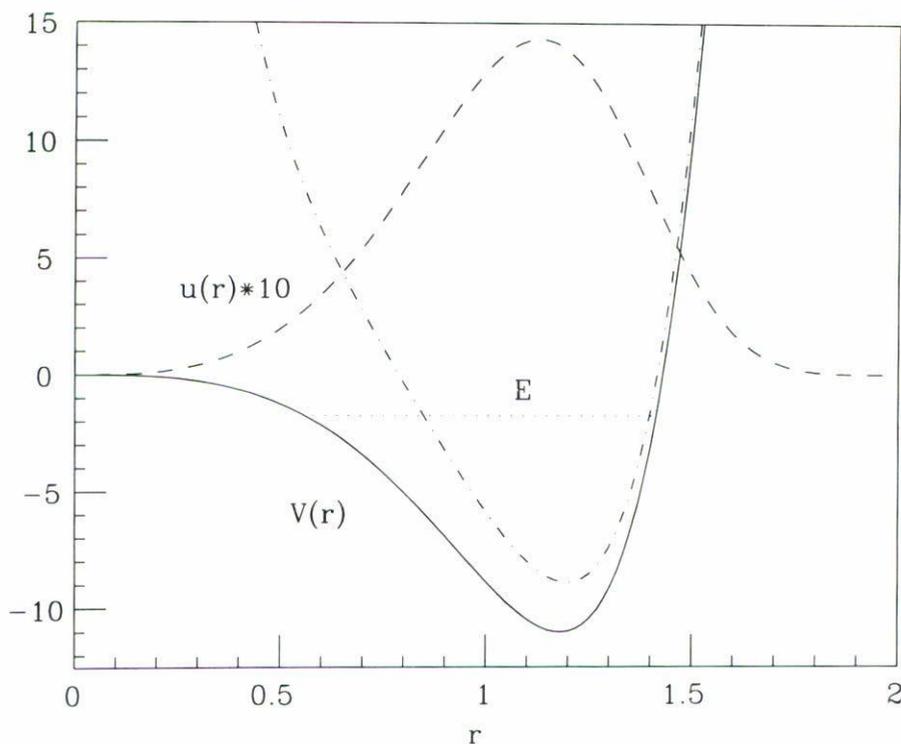


FIGURE 1. The potential  $0.125 r^2 - 10 r^3 - r^5 + 2r^8$  (solid line) and its associated effective potential including the effect of the centrifugal barrier (dot-dashed line) for  $l = 2$ . The  $1d$  reduced radial wave function  $u(r) \propto r^3 \exp(0.25 r^2 - 0.4 r^5)$  (dashed line) is also shown together with the corresponding energy level (dotted line).

while the matching procedure gives

$$\sqrt{2a_8} R^5 + \frac{a_5}{\sqrt{2a_8}} R^2 = l + 2, \tag{16}$$

which yields  $R = 1.1269$  for  $l = 1$ . It is interesting to note here that Eq. (16) has only one real and positive root. The energy eigenvalue for the potential (14) reads

$$E = \frac{2l + 5}{2} \frac{a_5}{\sqrt{2a_8}} - \frac{1}{2R^2} + \sqrt{2a_8} R^3. \tag{17}$$

The potential function and its associated effective potential are displayed in Fig. 2. Of course, since the “solvability conditions” (15) differ from those of Eq. (13), the potential of this figure is not identical to the one of Fig. 1. The radial wf for the  $2p$ -state is also depicted in Fig. 2.

Additional examples can be easily construed. For the sake of brevity, however, we shall content ourselves with the two instances discussed above.

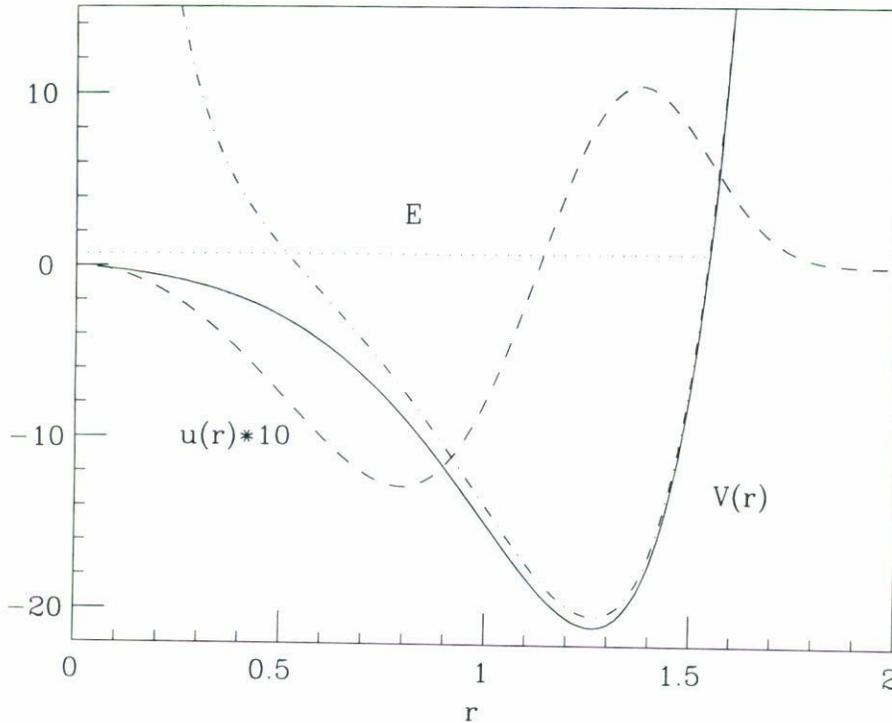


FIGURE 2. The potential  $-2.0962r - 2.1288r^2 - 10r^3 - 1.7747r^4 - r^5 + 2r^8$  (solid line) and its associated effective potential including the effect of the centrifugal barrier (dot-dashed line) for  $l = 1$ . The  $1p$  reduced radial wave function  $u(r) \propto r^2(r - 1.1269) \exp(0.8874r + 0.25r^2 - 0.4r^5)$  (dashed line) is also shown together with the corresponding energy level (dotted line).

#### 4. CONCLUDING REMARKS

Summing up, we have here presented a straightforward algorithm that allows the beginning student to try her (his) hand at determining, for general potentials of the type (3), the "solvability conditions" that provide for specific realizations leading to exact reduced radial wf of a quite simple form.

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