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ON THE CLASSICAL THEORY OF ORDINARY LINEAR DIFFERENTIAL EQUATIONS OF THE SECOND ORDER AND THE SCHRÖDINGER EQUATION FOR POWER LAW POTENTIALS

by

Marcia L. Lima* and Juan A. Mignaco

Centro Brasileiro de Pesquisas Físicas - CNPq/CBPF
Rua Dr. Xavier Sigaud, 150
22290 - Rio de Janeiro, RJ - Brasil

*Departamento de Física Teórica
Instituto de Física
Universidade Federal do Rio de Janeiro
21910 - Rio de Janeiro, RJ - Brasil

Abstract

The power law potentials in the Schrödinger equation solved recently are shown to come from the classical treatment of the singularities of a linear, second order differential equation. This allows to enlarge the class of solvable power law potentials.

Key-words: Powers law potentials; Singularities in Schroedinger equation.

Considerable attention has been drawn recently to the solutions of the Schrödinger equation for central power law potentials:

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

$$U(r) = \sum_{i=1}^{N} \gamma_i r^{\alpha_i} \qquad , \alpha_N : \text{rational number}$$

The set of exponents $\{\alpha_i\}$ forms in general an ordered sequence of equally spaced numbers including the powers for the energy and centrifugal terms.

In a series of articles(1-5) Znojil has set up a general procedure to obtain solutions to (1). In terms of classical texts(6)(7) the procedure proposes "normal" or "subnormal" solutions around the singular points at zero and infinity. Starting from the solutions for "confining" potentials(8) with $\alpha_i \geq 0$ a relation can be established with the solutions corresponding to several other sets $\{\alpha_i\}$. For confining potentials, one writes:

$$u_{k\ell}(r) = r^{\sigma} \exp\left[-f(r)\right] v_{k\ell}(r) \qquad (2)$$

with f(r) a polynomial and $v_{k\ell}$ an analytic function.

Znojil(1)(5) has shown that the solutions proposed, whose energy eigenvalues result from the Green's function, converge.

Examining the problem for confining potentials Znojil(2) and Rampal and Datta(9) have shown that in order to obtain polynomial solutions the coupling constants γ_i must satisfy some constraint equations. In general, it is not possible to fulfill these equations but only for certain sets $\{\alpha_i\}$.

Other authors[10] have also obtained different solutions which turn out to be special cases of those from the work by Znojil and Rampal and Datta.

In this work we wish to present another point of view on the same subject. This viewpoint is not totally new since it is based upon the classical theory of ordinary linear differential equations of the second order (an expression we shall abbreviate as OLDESO) proposed decades ago by Ince[6] and partly exploited by Bose[11] and Lemieux and Bose[12] in pioneer work not fully appreciated. We shall show how all cases treated in the literature mentioned above can be covered by the unifying classification proposed by Ince which allows also for new ones.

According to Ince all OLDESO might be classified in a scheme starting from original ones having different fixed numbers of elementary regular singularities. These are defined as singular points of the general equation

$$\frac{d^2w}{dz^2} + p(z)\,\frac{dw}{dz} + q(z)w = 0 \tag{3}$$

having exponents in its indicial equation which differ by 1/2. The coalescence of these elementary regular singularities gives rise to a new kind of singularity called regular if their exponents are two arbitrary numbers or irregular if it has a single exponent or none. A regular singularity comes from the coalescence of a pair of elementary regular ones, and an irregular singularity results when three or more of the ele mentary regular singularities are made to coincide. The order of an irregular singularity is j when it is originated from j+2 elementary regular singular points. In Ince's notation, an OLDESO may be classified as $[L,M,N_j + N_k + \ldots]$ where L is the number of elementary regular singularities, M is the number of regular ones, and N_j, N_k,... are the numbers of irregular singular points of kinds j,k,... .

Though details are given in chapter XX of Ince, let us recall that from $[2N,0,0]$ the coalescence of couples of elementary regular singularities carry onto a $[0,N,0]$ equation, which should be the solution of the generalized Riemann's problem[13]. The usual Riemann's problem with singularities at three points is N = 3, and the Whittaker[14] confluent equation is obtained from it as $[0,1,1_2]$.

From the physical point of view, the interesting cases seem to be those where in (1) the origin is at least a regular singular point (as long as the centrifugal term is present in (1)) and infinity is always an irregular singular point, since the energy term must be always in place. These singularities may be produced by coalescence of simpler ones but another mechanism[2-5] involves the use of transformations on the independent variable[15]. The combination of both artifacts leads to all cases analyzed and solved in the literature for equation (1) and also several not considered yet. This is the matter of our work.

The path to be followed was indicated by Bose[11] and Lemieux and Bose[12], and is also contained in the works of Ref. 15 and in the work by Znojil[2-5]. The substitution

$$w = y \exp\left[-\frac{1}{2}\int p(z')dz'\right] \tag{4}$$

brings (3) into its "normal" form

$$\frac{d^2y}{dz^2} + I(z)y = 0 \tag{5}$$

where I(z) is called the invariant of the normal form of the equation and is given by

$$I(z) = q(z) - \frac{1}{2}\frac{dp(z)}{dz} - \frac{1}{4}p^2(z) \quad . \tag{6}$$

Using a generalized transformation[11,12,15] the normal form is taken to a normal form of the Schrödinger equation, that is (1), having a constant (energy) term and a centrifugal one. The Schrödinger equation will be for f(x) related to y(z) through:

$$y(z) = \left(\frac{dz}{dx}\right)^{1/2} f(x) \tag{7a}$$

and the invariant for (1) becomes:

$$I^s(x) = \left(\frac{dz}{dx}\right)^2 I(z(x)) + \frac{1}{2}\{z,x\} \tag{7b}$$

where the last term is the Schwarz derivative

$$\{z,x\} = \left(\frac{dz}{dx}\right)^{-1}\left(\frac{d^3z}{dx^3}\right) - \frac{3}{2}\left[\left(\frac{dz}{dx}\right)^{-1}\left(\frac{d^2z}{dx^2}\right)\right]^2 \quad . \tag{7c}$$

The invariant $I^s(x)$ (or $I(z)$) contains all the information about the singularities of the equation.

In the table we exhibit for N = 3,4 and 5 the potentials which can be solved knowing one of them and making a transformation which is also indicated for an initial $[2N,0,0]$ kind of OLDESO. It is understood that the largest positive power and/or the smallest negative power in the potential must have a positive coefficient. We leave the details for a forthcoming publication and restrict to some comments.

For the case N = 3 we reproduce the results by Bose(11) for the confluences $[0,1,1_2]$ at zero and infinity, respectively; it is the well known Coulomb problem. Via $z = \alpha x^2$ it transforms into the equation for the harmonic oscillator. We incorporate another case, that starting from

$$I(z) = Az^{-3} + Bz^{-2} + Cz^{-1} \quad , \tag{8a}$$

corresponding to two irregular singularities of the first kind, $[0,0,2_1]$, at the origin and infinity; it goes into

$$I^s(x) = \frac{\gamma_1}{x^4} + \frac{\gamma_2}{x^2} + k^2 \tag{8b}$$

whose exact solutions have been studied by Spector(16). Notice that this is of a kind of confluences that do not derive from regular singularities, i.e., from $[0,3,0]$.

For N = 4 we have that $[0,4,0]$ corresponds to the equation proposed by Heun(17). Its polynomial solutions were studied by Erdélyi(18). The confluences starting from it have been considered by Maroni(19) and Pham Ngoc Dinh(20) and both proved the con vergence of their solutions. Lemieux and Bose studied Heun's equation and its confluences $[0,1,1_2]$ and $[0,0,2_2]$. In our table we exhibit also the case $[0,0,1_1+1_3]$ which does not belong neither to the cases considered by Znojil[2-5].

For N = 5, the pattern of confluences reproduces, and now we have two new cases not considered before: the families for $[0,0,1_1+1_5]$ and $[0,0,2_3]$. Notice that the former contains the well known Lennard-Jones potential used currently in molecular physics.

Whereas the singularities produced from $[0,N,0]$ are the ones studied by Znojil and previous authors, the others are considered for a moment by Rampal and Datta[9]. These authors have shown that they can receive the same treatment proposed by Znojil but they admit no polynomial solutions. Incidentally, the polynomial solutions by Rampal and Datta can be obtained from the articles by Maroni[19] and Dinh[20].

Notice that the transformations studied by Johnson[15] can scarcely have any meaning outside the group of solutions proposed here, since otherwise the remaining singularity at infinity causes troubles.

We may show (and shall do it in a forthcoming article) that a number of other potentials can be considered as long as we consider other transformations of variable than power like.

Lemieux and Bose[12] showed how $[0,4,0]$ might copy a two-center potential, such as the Coulomb potential in the hydrogen ionized molecule H_2^+. We believe that multi-center potentials may equally come out of the case $[0,N,0]$ $(N > 4)$.

What about the equations coming from $[2N+1,0,0]$? One can apply similar procedures to those outlined above, but clearly the point is that here always one singularity comes from an odd number of elementary regular ones. The potentials arising from [2N+1,0,0] somehow fill gaps in our table, giving rise for instance to forms like

$$I^s(x) = \frac{\gamma_1}{x^2} + \frac{\gamma_2}{x} + k^2 + \gamma_3 x \tag{9}$$

For these potentials, as remarked by Rampal and Datta(9), no polynomial solutions can be found.

One may raise the question whether all potential forms may be obtained and solved this way. At first sight, there are no means to include a potential with an irrational power, and is not evident either that any OLDESO might be solved by a normal solution.

Summarizing, the classical theory of OLDESO together with the normal solutions proposed by Znojil are able to solve an enormous variety of potentials, many of physical interest, for the two body forces. It will continue to provide an important tool for the understanding of potential theory.

TABLE

POTENTIALS GENERATED FROM $[2N,0,0]$ BY CONFLUENCE

N = 3

Confluence: $[0,1,1_2]$; Invariant: $I(z) = \frac{A}{z^2} + \frac{B}{z} + c$

Schrödinger invariants:	Transformations:
$I^s(r) = \gamma_1 r^{-2} + \gamma_2 r^{-1} + k^2$	$z = \alpha r$
$I^s(r) = \gamma_1 r^{-2} + k^2 + \gamma_2 r^2$	$z = \alpha r^2$

Confluence: $[0,0,2_1]$; Invariant: $I(z) = \frac{A}{z^3} + \frac{B}{z^2} + \frac{C}{z}$

$I^s(r) = \gamma_1 r^{-4} + \gamma_2 r^{-2} + k^2$	$z = \alpha r^2$

N = 4

Confluence: $[0,1,1_4]$; Invariant: $I(z) = \frac{A}{z^2} + \frac{B}{z} + C + Dz + Ez^2$

Schrödinger invariants:	Transformations:
$I^s(r) = \gamma_1 r^{-2} + \gamma_2 r^{-3/2} + \gamma_3 r^{-1} + \gamma_4 r^{-1/2} + k^2$	$z = \alpha r^{1/2}$
$I^s(r) = \gamma_1 r^{-2} + \gamma_2 r^{-4/3} + \gamma_3 r^{-2/3} + k^2 + \gamma_4 r^{2/3}$	$z = \alpha r^{2/3}$
$I^s(r) = \gamma_1 r^{-2} + \gamma_2 r^{-1} + k^2 + \gamma_3 r + \gamma_4 r^2$	$z = \alpha r$
$I^s(r) = \gamma_1 r^{-2} + k^2 + \gamma_2 r^2 + \gamma_3 r^4 + \gamma_4 r^6$	$z = \alpha r^2$

Confluence: $[0,0,1_2+1_3]$; Invariant: $I(z) = \frac{A}{z^3} + \frac{B}{z^2} + \frac{C}{z} + D + Ez$

Schrödinger invariants:	Transformations:
$I^s(r) = \gamma_1 r^{-8/3} + \gamma_2 r^{-2} + \gamma_3 r^{-4/3} + \gamma_4 r^{-2/3} + k^2$	$z = \alpha r^{2/3}$
$I^s(r) = \gamma_1 r^{-3} + \gamma_2 r^{-2} + \gamma_3 r^{-1} + k^2 + \gamma_4 r$	$z = \alpha r$
$I^s(r) = \gamma_1 r^{-4} + \gamma_2 r^{-2} + k^2 + \gamma_3 r^2 + \gamma_4 r^4$	$z = \alpha r^2$
$I^s(r) = k^2 + \gamma_1 r^{-2} + \gamma_2 r^{-4} + \gamma_3 r^{-6} + \gamma_4 r^{-8}$	$z = \alpha r^{-2}$

Confluence: $[0,0,2_2]$; Invariant: $I(z) = \frac{A}{z^4} + \frac{B}{z^3} + \frac{C}{z^2} + \frac{D}{z} + E$

Schrödinger invariants:	Transformations:
$I^s(r) = \gamma_1 r^{-4} + \gamma_2 r^{-3} + \gamma_3 r^{-2} + \gamma_4 r^{-1} + k^2$	$z = \alpha r$
$I^s(r) = \gamma_1 r^{-6} + \gamma_2 r^{-4} + \gamma_3 r^{-2} + k^2 + \gamma_4 r^2$	$z = \alpha r^2$

N = 5

Confluence: $[0,1,1_6]$; Invariant: $I(z) = \frac{A}{z^2} + \frac{B}{z} + C + Dz + Ez^2 + Fz^3 + Gz^4$

Schrödinger invariants: Transformations:

$$I^s(r) = \gamma_1 r^{-2} + \gamma_2 r^{-5/3} + \gamma_3 r^{-4/3} + \gamma_4 r^{-1} + \gamma_5 r^{-2/3} + \gamma_6 r^{-1/3} + k^2 \qquad z = \alpha r^{-1/3}$$

$$I^s(r) = \gamma_1 r^{-2} + \gamma_2 r^{-8/5} + \gamma_3 r^{-6/5} + \gamma_4 r^{-4/5} + \gamma_5 r^{-2/5} + k^2 + \gamma_6 r^{2/5} \qquad z = \alpha r^{2/5}$$

$$I^s(r) = \gamma_1 r^{-2} + \gamma_2 r^{-3/2} + \gamma_3 r^{-1} + \gamma_4 r^{-1/2} + k^2 + \gamma_5 r^{1/2} + \gamma_6 r \qquad z = \alpha r^{1/2}$$

$$I^s(r) = \gamma_1 r^{-2} + \gamma_2 r^{-4/3} + \gamma_3 r^{-2/3} + k^2 + \gamma_4 r^{2/3} + \gamma_5 r^{4/3} + \gamma_6 r^2 \qquad z = \alpha r^{2/3}$$

$$I^s(r) = \gamma_1 r^{-2} + \gamma_2 r^{-1} + k^2 + \gamma_3 r + \gamma_4 r^2 + \gamma_5 r^3 + \gamma_6 r^4 \qquad z = \alpha r$$

$$I^s(r) = \gamma_1 r^{-2} + k^2 + \gamma_2 r^2 + \gamma_3 r^4 + \gamma_4 r^6 + \gamma_5 r^8 + \gamma_6 r^{10} \qquad z = \alpha r^2$$

Confluence: $[0,0,1_1+1_5]$; Invariant: $I(z) = \frac{A}{z^3} + \frac{B}{z^2} + \frac{C}{z} + D + Ez + Fz^2 + Gz^3$

Schrödinger invariants: Transformations:

$$I^s(r) = \gamma_1 r^{-12/5} + \gamma_2 r^{-2} + \gamma_3 r^{-8/5} + \gamma_4 r^{-6/5} + \gamma_5 r^{-4/5} + \gamma_6 r^{-2/5} + k^2 \qquad z = \alpha r^{2/5}$$

$$I^s(r) = \gamma_1 r^{-5/2} + \gamma_2 r^{-2} + \gamma_3 r^{-3/2} + \gamma_4 r^{-1} + \gamma_5 r^{-1/2} + k^2 + \gamma_6 r^{1/2} \qquad z = \alpha r^{1/2}$$

$$I^s(r) = \gamma_1 r^{-8/3} + \gamma_2 r^{-2} + \gamma_3 r^{-4/3} + \gamma_4 r^{-2/3} + k^2 + \gamma_5 r^{2/3} + \gamma_6 r^{4/3} \qquad z = \alpha r^{2/3}$$

$$I^s(r) = \gamma_1 r^{-3} + \gamma_2 r^{-2} + \gamma_3 r^{-1} + k^2 + \gamma_4 r + \gamma_5 r^2 + \gamma_6 r^3 \qquad z = \alpha r$$

$$I^s(r) = \gamma_1 r^{-4} + \gamma_2 r^{-2} + k^2 + \gamma_3 r^2 + \gamma_4 r^4 + \gamma_5 r^6 + \gamma_6 r^8 \qquad z = \alpha r^2$$

$$I^s(r) = k^2 + \gamma_1 r^{-2} + \gamma_2 r^{-4} + \gamma_3 r^{-6} + \gamma_4 r^{-8} + \gamma_5 r^{-10} + \gamma_6 r^{-12} \qquad z = \alpha r^{-2}$$

Confluence: $[0,0,1_2+1_4]$; Invariant: $I(z) = \frac{A}{z^4} + \frac{B}{z^3} + \frac{C}{z^2} + \frac{D}{z} + E + Fz + Gz^2$

Schrödinger invariants: Transformations:

$$I^s(r) = \gamma_1 r^{-3} + \gamma_2 r^{-5/2} + \gamma_3 r^{-2} + \gamma_4 r^{-3/2} + \gamma_5 r^{-1} + \gamma_6 r^{-1/2} + k^2 \qquad z = \alpha r^{1/2}$$

$$I^s(r) = \gamma_1 r^{-10/3} + \gamma_2 r^{-8/3} + \gamma_3 r^{-2} + \gamma_4 r^{-4/3} + \gamma_5 r^{-2/3} + k^2 + \gamma_6 r^{2/3} \qquad z = \alpha r^{2/3}$$

$$I^s(r) = \gamma_1 r^{-4} + \gamma_2 r^{-3} + \gamma_3 r^{-2} + \gamma_4 r^{-1} + k^2 + \gamma_5 r + \gamma_6 r^2 \qquad z = \alpha r$$

$$I^s(r) = \gamma_1 r^{-6} + \gamma_2 r^{-4} + \gamma_3 r^{-2} + k^2 + \gamma_4 r^2 + \gamma_5 r^4 + \gamma_6 r^6 \qquad z = \alpha r^2$$

$$I^s(r) = \gamma_1 r^2 + k^2 + \gamma_2 r^{-2} + \gamma_3 r^{-4} + \gamma_4 r^{-6} + \gamma_5 r^{-8} + \gamma_6 r^{-10} \qquad z = \alpha r^{-2}$$

$$I^s(r) = k^2 + \gamma_1 r^{-1} + \gamma_2 r^{-2} + \gamma_3 r^{-3} + \gamma_4 r^{-4} + \gamma_5 r^{-5} + \gamma_6 r^{-6} \qquad z = \alpha r^{-1}$$

Confluence $[0,0,2_3]$; Invariant: $I(z) = \frac{A}{z^5} + \frac{B}{z^4} + \frac{C}{z^3} + \frac{D}{z^2} + \frac{E}{z} + F + Gz$

Schrödinger invariants: Transformations:

$$I^s(r) = \gamma_1 r^{-4} + \gamma_2 r^{-10/3} + \gamma_3 r^{-8/3} + \gamma_4 r^{-2} + \gamma_5 r^{-4/3} + \gamma_6 r^{-2/3} + k^2 \qquad z = \alpha r^{2/3}$$

$$I^s(r) = \gamma_1 r^{-5} + \gamma_2 r^{-4} + \gamma_3 r^{-3} + \gamma_4 r^{-2} + \gamma_5 r^{-1} + k^2 + \gamma_6 r \qquad z = \alpha r$$

$$I^s(r) = \gamma_1 r^{-8} + \gamma_2 r^{-6} + \gamma_3 r^{-4} + \gamma_4 r^{-2} + k^2 + \gamma_5 r^2 + \gamma_6 r^4 \qquad z = \alpha r^2$$

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