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Several Remarks on Exact Solutions of One-Particle Equations *

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Abstract. Semi-exact, quasi-exact and conditionally-exact solutions of one-particle equations are discussed. In particular, symmetry conditions under which the Klein-Gordon and the Dirac equations are reducible to Schrödinger-like form and, thus, the exact solubility of the Schrödinger equation implies that its relativistic counterparts are also exactly solvable, are discussed. Another problem addressed in this report is the semi-exact, quasi-exact and conditionally-exact solubility of the radial Schrödinger equations with power potentials. The equations are shown to be semi-exactly solvable with solutions expressible in terms of the Hessenberg determinants. Conditions under which quasi-exact solutions exist are also presented.

1 Introduction

Usually one-particle eigenvalue problems have to be solved numerically. Several exactly solvable cases, as for example harmonic oscillator or hydrogen atom, play an important role in many branches of quantum mechanics. Quasi-exactly solvable equations, where a finite number of solutions (usually just one) may be expressed analytically, have been intensively studied over last two decades [1,2]. The best known example is the *Hooke atom*, also known as *harmonium* [3, 4]. For equations referred to as *conditionally-exactly-solvable* analytic solutions may be obtained for specific values of the potential parameters [5]. Finally, in the case of *semi-exactly-solvable* equations the wave functions may be expressed analytically, but the eigenvalues have to be derived numerically [6, 7].

In the relativistic case, the Dirac and the Klein-Gordon equations may be conditionally reduced to a form analogous to the Schrödinger equation [8]. As discussed in the next section, the relativistic equations with electrostatic component of the vector potential equal to the scalar part of the potential, *i.e.*equations describing systems with spin symmetry [9], are always reducible to a Schrödinger like-equation with the energy-dependent effective mass [10].

One-particle potentials expressed as polynomials of the radial variable are known as the *power potentials*. In the third section it is demonstrated that the Schrödinger equations with power potentials are semi-exactly-solvable and their

*This work is dedicated to the memory of Dr. Rossen Lubenov Pavlov solutions may be expressed in terms of the Hessenberg determinants [7, 11]. Conditions under which the equations with power potentials are either exactly or quasi-exactly solvable are also presented [12].

Finally, in the last section, some examples of semi-exact solutions are briefly discussed.

2 Relativistic Equations with Spin Symmetry

Let us consider a relativistic particle in the field of an electrostatic potential V_e and a scalar potential V_s. A spinless particle is described by the Klein-Gordon equation:

$$\left[\mathsf{p}^2\, c^2 + (mc^2 + \mathsf{V}_\mathrm{s})^2 - (E - \mathsf{V}_\mathrm{e})^2\right] \Psi(\boldsymbol{r}) = 0, \tag{1}$$

where all symbols have their usual meaning. After some simple rearrangement, the equation may be rewritten as

$$\left[\frac{\mathsf{p}^2}{2m} + (\mathsf{V}_\mathrm{e} + \mathsf{V}_\mathrm{s}) \left(1 - \frac{\mathsf{V}_\mathrm{e} - \mathsf{V}_\mathrm{s}}{2mc^2}\right) + \frac{\mathcal{E}\,\mathsf{V}_\mathrm{e}}{mc^2} - \mathcal{E}\left(1 + \frac{\mathcal{E}}{2mc^2}\right)\right] \Psi(\boldsymbol{r}), \tag{2}$$

where $\mathcal{E} = E - mc^2$. If we set $\mathsf{V}_\mathrm{e} = \mathsf{V}_\mathrm{s} = \mathsf{V}/2$, then (2) transforms to a Schrödinger-like equation:

$$\left[\frac{\mathsf{p}^2}{2\mathfrak{M}} + \mathsf{V} - \mathcal{E}\right] \Psi(\boldsymbol{r}) = 0, \tag{3}$$

where*

$$\mathfrak{M} \equiv \mathfrak{M}(\mathcal{E}) = m\left(1 + \frac{\mathcal{E}}{2mc^2}\right). \tag{4}$$

A spin-$1/2$ fermion is described by the Dirac equation

$$\begin{bmatrix} \left(\mathsf{V}_\mathrm{e} + \mathsf{V}_\mathrm{s} + mc^2 - E\right) I_2 & c\,(\boldsymbol{\sigma}\cdot\boldsymbol{p}) \\ c\,(\boldsymbol{\sigma}\cdot\boldsymbol{p}) & \left(\mathsf{V}_\mathrm{e} - \mathsf{V}_\mathrm{s} - mc^2 - E\right) I_2 \end{bmatrix} \begin{bmatrix} \Psi_\mathrm{L}(\boldsymbol{r}) \\ \Psi_\mathrm{S}(\boldsymbol{r}) \end{bmatrix} = 0, \tag{5}$$

where I_2 is 2×2 unit matrix. Taking $\mathsf{V}_\mathrm{e} = \mathsf{V}_\mathrm{s}$, after some simple algebra, we can separate the equations for the large (upper) and the small (lower) component:

$$\left[\frac{(\boldsymbol{\sigma}\cdot\boldsymbol{p})^2}{2\mathfrak{M}} + \mathsf{V} - \mathcal{E}\right] \Psi_\mathrm{L}(\boldsymbol{r}) = 0, \tag{6}$$

$$\Psi_\mathrm{S}(\boldsymbol{r}) = \frac{(\boldsymbol{\sigma}\cdot\boldsymbol{p})}{2\mathfrak{M}c}\,\Psi_\mathrm{L}(\boldsymbol{r}), \tag{7}$$

Since $(\boldsymbol{\sigma}\cdot\boldsymbol{p})^2 = \boldsymbol{p}^2\, I_2$, solutions of (6) may be expressed in terms of solutions of (3):

$$\Psi_\mathrm{L}(\boldsymbol{r}) = \left[c_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + c_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right] \Psi(\boldsymbol{r}), \tag{8}$$

*Some intuitive meaning of $\mathfrak{M}$ can be derived from the observation that the relativistic energy-momentum relation $E^2 = (mc^2)^2 + (pc)^2$, for $E > mc^2$, can be rewritten as $\mathcal{E} = p^2/(2\mathfrak{M})$.

with $|c_1|^2 + |c_2|^2 = 1$.

Let us note, that the energy spectra E of (3) and (6) are positive and bounded from below. The non-relativistic limits may be obtained in a straightforward way by setting $\mathfrak{M} = m$. The discussion of the negative energy solutions is beyond the scope of this report. An interested reader is referred to, *e.g.*, [8].

Let $\mathcal{E}^{\mathrm{Sh}}[m]$ be an eigenvalue of the Schrödinger Hamiltonian for a particle with mass m

$$\left[\frac{\mathsf{p}^2}{2m} + \mathsf{V} - \mathcal{E}^{\mathrm{Sh}}[m]\right] \Psi^{\mathrm{Sh}}(\boldsymbol{r}) = 0. \tag{9}$$

By comparing (9) and (3) one can see that

$$\mathcal{E} = \mathcal{E}^{\mathrm{Sh}}[\mathfrak{M}(\mathcal{E})]. \tag{10}$$

The explicit expression for $\mathcal{E}$ may be obtained by solving (10) with respect to $\mathcal{E}$. A similar procedure may be applied to the wave-functions. Thus, if the solution of the Schrödinger equation is known, then the corresponding solution of either Klein-Gordon or Dirac equation with spin symmetry may be obtained by some algebraic manipulation.

In some cases the mass-dependence of the Schrödinger energies is particularly simple. For example, if $\mathsf{V} = r^n$, where $r = |\boldsymbol{r}|$ then, as one can see by the application of a scaling procedure,

$$\mathcal{E}^{\mathrm{Sh}}[m] = m^{-n/(n+2)} \mathcal{E}^{\mathrm{Sh}}[1]. \tag{11}$$

Then, in this case (10) can be rewritten as

$$\mathcal{E} \left(1 + \frac{\mathcal{E}}{2mc^2}\right)^{n/(n+2)} = \mathcal{E}^{\mathrm{Sh}}[m]. \tag{12}$$

In particular, for the Coulomb potential $n = -1$. Consequently, the energy levels of a relativistic particle with spin symmetry in the central Coulomb field are given by the following formula

$$\mathcal{E} = \frac{\mathcal{E}^{\mathrm{Sh}}[m]}{1 - \mathcal{E}^{\mathrm{Sh}}[m]/(2mc^2)}. \tag{13}$$

After the substitution of $\mathcal{E}^{\mathrm{Sh}}[m] = -mZ^2e^4/(2n^2\hbar^2)$ we get

$$\mathcal{E} = \frac{-m\, Z^2 e^4}{2n^2\hbar^2 + Z^2e^4/2c^2}, \tag{14}$$

equivalent to equation (3.4) of reference [8].

3 Schrödinger Equation with Power Potentials

In this section we are concerned with solutions of the radial Schrödinger equation

$$\left[\frac{\mathsf{p}^2}{2m} + \mathsf{V}(r) - \mathcal{E}\right] \Psi(r, \theta, \phi) = 0, \tag{15}$$

where V is a power potential. After the elimination of the angular part, the equation may be rewritten in the *normal form*

$$\left[\frac{d^2}{dr^2} - \mathsf{W}(r)\right]\psi(r) = 0. \tag{16}$$

In order to simplify our analysis we assume that

$$\mathsf{W}(r) = \sum_{j=-2}^{\mathsf{N}} \alpha_j\, r^j, \tag{17}$$

with $N = 2m$ - an even integer, and $\alpha_{\mathsf{N}} > 0$. A discussion of the case of the odd N may be found in [7]. A study on the potentials with $\alpha_{\mathsf{N}} < 0$, when the bound-state solutions do not exist, suggested to the author by by Hitoshi Nakada during a discussion at the Workshop, will be presented elsewhere.

It is convenient to express the radial wave-function in the form

$$\psi(r) = F_0(r)\, P(r)\, F_\infty(r), \tag{18}$$

where F_0 and F_∞ are derived directly from the form of the potential to describe the asymptotic behavior of the solutions at $r \to 0$ and $r \to \infty$, respectively, and

$$P(r) = \sum_{n=0}^{\infty} a_n\, r^n. \tag{19}$$

We select the asymptotic factors corresponding to the regular (square-integrable) solutions if $P(r)$ doesnot influence the asymptotic behavior of $\psi(r)$. After some standard algebra we get:

$$F_0(r) \;=\; r^{\lambda+1}, \quad \lambda = \pm\sqrt{\frac{1}{4} + \alpha_{-2}} - \frac{1}{2}, \tag{20}$$

where the positive root corresponds to the solutions regular at $r \to 0$,

$$F_\infty(r) \;= \mathsf{e}^{-\eta(r)}, \quad \eta(r) = \sum_{n=1}^{m+1} \frac{\beta_n}{n}\, r^n, \tag{21}$$

where

$$\begin{aligned} \beta_{m+1} &= \sqrt{\alpha_{\mathrm{N}}}, \\ \beta_{m+1-k} &= \frac{1}{2\beta_{m+1}}\left[\alpha_{2m-k} - \sum_{i=1}^{k-1} \beta_{i+m-k+1}\beta_{m-i+1}\right], \\ & \quad k = 1, 2, \ldots, m. \end{aligned} \tag{22}$$

The substitution to the original equation results in an $(m+2)$-term recurrence relation defining the expansion coefficients [7]:

$$a_{n+1} = \sum_{j=0}^{m} g_{n-j}^{(j)} a_{n-j}. \tag{23}$$

Since $a_k = 0$ for $k < 0$, we have $g_k^{(j)} = 0$ if $k < 0$. For $k \geq 0$,

$$g_k^{(j)} = \frac{(2k + j + 2\lambda + 2)\beta_{j+1} - \sum_{i=1}^{j} \beta_i \beta_{j-i+1} + \alpha_{j-1}}{(k + j + 1)(k + j + 2\lambda + 2)}. \tag{24}$$

The normalization condition $P(0) = a_0 = 1$ has been assumed.

If the recurrence (24) terminates then $P(r)$ is a polynomial and the wavefunction may be expressed analytically as the product (18) of the polynomial and the asymptotic factors. These solutions are referred to as the *polynomial solutions*. Most of square-integrable solutions are *non-polynomial*. One can show [7, 11, 12] that for the power potentials with even maximum power N one can always select the parameters of $\mathsf{W}(r)$ in such a way that a polynomial solution (usually one) exists. It is surprising that for odd N polynomial solutions do not exist [7].

3.1 Hessenberg determinants

Square band matrices with upper bandwidth equal to 1 and the lower bandwidth equal to u are referred to as lower Hessenberg matrices [13]. We are concerned with a special kind of these matrices in which the super-diagonal elements are equal to -1. We denote the Hessenberg matrix as

$$\mathbb{M}_n^{(u)}(\mathbf{G}) \equiv \mathbb{M}_n^{(u)}(\mathbb{G}_0, \mathbb{G}_1, \ldots, \mathbb{G}_u) \tag{25}$$

where

$$\mathbb{G}_0 = \left[g_0^{(0)}, g_1^{(0)}, \ldots, g_n^{(0)}\right]$$

is the diagonal and the sub-diagonals are

$$\mathbb{G}_j = \left[g_0^{(j)}, g_1^{(j)}, \ldots, g_{n-j}^{(j)}\right], \quad j = 1, 2, \ldots, u.$$

For example, if $n = 6$ and $u = 2$ then

$$\mathbb{M}_6^{(2)}(\mathbf{G}) = \begin{bmatrix} g_0^{(0)} & -1 & 0 & 0 & 0 & 0 \\ g_0^{(1)} & g_1^{(0)} & -1 & 0 & 0 & 0 \\ g_0^{(2)} & g_1^{(1)} & g_2^{(0)} & -1 & 0 & 0 \\ 0 & g_1^{(2)} & g_2^{(1)} & g_3^{(0)} & -1 & 0 \\ 0 & 0 & g_2^{(2)} & g_3^{(1)} & g_4^{(0)} & -1 \\ 0 & 0 & 0 & g_3^{(2)} & g_4^{(1)} & g_5^{(0)} \end{bmatrix},$$

$$\mathsf{G} = [\mathbb{G}_0, \mathbb{G}_1, \mathbb{G}_2]$$

Determinant of the Hessenberg matrix is named the Hessenberg determinant and denoted $M_n^{(u)}(\mathsf{G})$.

3.2 Semi-exact solutions

By using the Laplace formula, one can easily demonstrate that the Hessenberg determinants fulfill the same recurrence relation as the coefficients of the expansion (19) of $P(r)$. Then we have

$$M_{n+1}^{(m)}(\mathsf{G}) = \sum_{j=0}^{m} g_{n-j}^{(j)} M_{n-j}^{(m)}(\mathsf{G}) \tag{26}$$

with

$$\mathsf{G} = [\mathbb{G}_0, \mathbb{G}_1, \ldots, \mathbb{G}_m] \,.$$

The recurrence relations (23) and (26) define, respectively, a_n and $M_n^{(m)}$ in a unique way (in both recurrences we set the same initial conditions, *i.e.* $a_0 = M_0 = 1$ and $a_k = M_k = 0$ if $k < 0$. Thus, we conclude that

$$a_n = M_n^{(m)}. \tag{27}$$

Since the elements of the determinants are defined in (24), we got explicit analytical expressions for the expansion coefficients of $P(r)$ and, consequently, explicit expression for the formal solution (18) of the Schrödinger equation [7]. The solutions are square integrable only if the values of $\mathcal{E}$ ere equal to the eigenvalues of the Hamiltonian. Therefore our solutions are *semi-exact* - we know the analytical form of the wave-function, however the energies have to be determined separately (the solutions corresponding to the values of the parameter $\mathcal{E}$ which are not equal to the Hamiltonian eigenvalues are not square integrable).

4 Examples

The number of terms in the recurrence relations (23) and (26) is determined by the highest power of r in the power potential. Thus, if $\mathsf{N} = 0$ we have two-term recurrences. They define *exactly solvable* hypergeometric equations. The quantization condition for $\mathcal{E}$ terminates the recurrence. The best known example is the hydrogen atom. Three-term recurrences correspond to the potentials with $\mathsf{N} = 2$. They define *quasi-exactly* and *semi-exactly* solvable Heun equations. The polynomial solutions are obtained if $\mathcal{E}$ and one parameter in the potential are properly constrained. The harmonium (the Hooke atom) and the shifted harmonic oscillator belong to the most commonly known examples. In a general case of an even N we have $\mathsf{N}/2 + 2$-term recurrences. For the polynomial solutions $\mathcal{E}$ and $\mathsf{N}/2$ parameters in the potential have to be constrained. In general the equations are semi-exactly solvable.

4.1 Two-term recurrence ($\mathsf{N}=0$)

In this case the Schrödinger equation is exactly solvable, the condition of termination of the recurrence defines the Hamiltonian eigenvalues and all bound states are described by the polynomial solutions. We have $m=0$,

$$\mathsf{W}(r)=\frac{\alpha_{-2}}{r^2}+\frac{\alpha_{-1}}{r}+\alpha_0, \tag{28}$$

$\eta = r\sqrt{\alpha_0}$, (23) is reduced to $a_{n+1}=g_n^{(0)}a_n$ with $a_0=1$ and

$$g_n^{(0)}=\frac{2(n+\lambda+1)\sqrt{\alpha_0}+\alpha_{-1}}{(n+1)(n+2\lambda+2)}. \tag{29}$$

The recurrence terminates at $n=p$ if $g_p^{(0)}=0$, *i.e.*if

$$\sqrt{\alpha_0}=\frac{-\alpha_1}{2(p+\lambda+1)}. \tag{30}$$

According to (27),

$$a_n=M_n^{(0)}=\begin{bmatrix} g_0^{(0)} & -1 & 0 & \cdots & 0 \\ 0 & g_1^{(0)} & -1 & \cdots & 0 \\ 0 & 0 & g_2^{(0)} & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & -1 \\ 0 & 0 & 0 & 0 & g_{n-1}^{(0)} \end{bmatrix} \tag{31}$$

and the radial wave-function (18) corresponding to n=p may be expressed in a compact form

$$\psi_p(r)=r^{\lambda+1}\begin{bmatrix} r^0 & r^1 & r^2 & \cdots & r^{p-1} & r^p \\ g_0^{(0)} & -1 & 0 & \cdots & 0 & 0 \\ 0 & g_1^{(0)} & -1 & \cdots & 0 & 0 \\ 0 & 0 & g_2^{(0)} & \ddots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & -1 & 0 \\ 0 & 0 & 0 & 0 & g_{p-1}^{(0)} & -1 \end{bmatrix}\mathrm{e}^{-r\sqrt{\alpha_0}}. \tag{32}$$

The Laplace formula, implies that the determinant is equal to $\sum_{n=0}^{p} a_n r^n$.

In the case of a hydrogen-like atom $\alpha_{-2}=l(l+1)$, $\lambda=l$, $\alpha_{-1}=-2Z$ and $\alpha_0=-2\mathcal{E}$. Equation (30) transforms to the hydrogenic energy formula and from (32) one can extract the determinantal representation of the Laguerre polynomial $L_{p+2l+1}^{2l+1}(\rho)$, where $\rho=2Z/(p+l+1)$.

4.2 Three-term recurrence ($\mathsf{N}=2$)

In this case the radial Schrödinger equation is the same as the normal form of the biconfluent Heun equation [14]. It may be obtained in the process of solving the problem of three-particle Hooke'an systems [2]. The Hooke atom (harmonium), received much attention starting from the seminal work by Kestner and Sinanoğlu [15] who noticed in 1962 that the Schrödinger for two electrons interacting by Coulomb forces and confined in a central harmonic potential is separable. Soon after Santos [16] demonstrated that the problem is quasi-exactly solvable. The results of Santos, unnoticed for several decades, have been rediscovered by Taut [3] and is mostly linked to his name. The structure of the energy spectrum of harmonium has been studied in [4].

It is convenient to express $\mathsf{W}(r)$ in the form

$$\mathsf{W}(r)=\frac{\lambda(\lambda+1)}{r^2}+\frac{z}{r}+\omega^2(r-r_0)^2-2\mathcal{E}. \tag{33}$$

Then $\alpha_{-2}=\lambda(\lambda+1)$, $\alpha_{-1}=z$, $\alpha_0=(\omega\, r_0)^2-2\mathcal{E}$, $\alpha_1=-2\omega^2 r_0$, $\alpha_2=\omega^2$, $\beta_1=-r_0/\omega$, $\beta_2=\omega$, $\eta=\omega\, r\,(r/2-r_0)$. The three-term recurrence relation reads

$$a_{n+1}=g_n^{(0)}\,a_n+g_{n-1}^{(1)}\,a_{n-1} \tag{34}$$

and

$$g_n^{(0)} = \frac{z-2\omega r_0(n+\lambda+1)}{(n+1)(n+2\lambda+2)} \tag{35}$$

$$g_n^{(1)} = \frac{-2\mathcal{E}+2\omega(n+\lambda+3/2)}{(n+2)(n+2\lambda+3)}. \tag{36}$$

For the polynomial solution the recurrence (34) has to terminate. Assume that $a_n\neq 0$ for $n=p$ and $a_n=0$ if $n>p$. After a simple analysis we can see that this requirement implies two conditions:

$$(1):\qquad g_p^{(1)}=0,\ \ \textit{i.e.}\ \ \mathcal{E}=\omega(p+\lambda+3/2), \tag{37}$$

$$(2):\qquad M_{p+1}^{(1)}(\mathbb{G}_0,\mathbb{G}_1)=0. \tag{38}$$

The second condition defines a relation between the parameters in W. For example, assuming for simplicity $r_0=0$, condition (2) for $p=1$ implies

$$g_0^{(0)}g_1^{(0)}+g_0^{(1)}=0 \quad\Rightarrow\quad z^2=4\omega(\lambda+1)$$

For $p=2$ we have

$$g_0^{(0)}g_1^{(0)}g_2^{(0)}+g_0^{(0)}g_1^{(1)}+g_2^{(0)}g_0^{(1)}=0$$

and, after some simple algebra, $z=0$ or $z^2=4\omega(4\lambda+5)$. More detailed analysis may be found in [17, 18].

As we see, the polynomial solutions exist for a specific set of the potential parameters. In general, for a given value of p there exits one set of such parameters (except for the cases of multiple solutions of the algebraic equations). This means that for each p we have at most several polynomial solutions. The remaining square-integrable solutions are non-polynomial *i.e.*the recurrence relation defining coefficients a_n, $n = 1, 2, \ldots \infty$ does not terminate. The convergence may be obtained only for the *exact* eigenvalues $\mathcal{E}$. Since these eigenvalues can only be derived with a finite accuracy, the expansion (19) has an asymptotic character and the best approximation is obtained if it is cut at a certain value of n.

5 Conclusions

- Relativistic Klein-Gordon and Dirac equations with spin symmetry are reducible to a Schrödinger like equation with energy-dependent mass. Consequently, the equations are exactly (quasi-exactly, semi-exactly, conditionally-exactly) solvable if the corresponding Schrödinger equation is exactly, etc., solvable.
- The Schrödinger equation with an arbitrary power potential is semi-exactly solvable and the solutions may be expressed as power series with coefficients equal to the Hessenberg determinants.
- Square-integrable wave-functions may be obtained by the substitution of the appropriate energy values to the general solutions. Since the energy eigenvalues are represented by finite strings of digits, the expansions are, in fact, asymptotic series.
- For potentials with an even maximum power of r the polynomial solutions exist if the parameters in the potential fulfill certain conditions. Schrödinger equations with odd-maximum-power potentials do not have polynomial solutions.
- The presented approach may be generalized to other forms of potentials.

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