EXACT SOLUTIONS OF THE SCHRÖDINGER EQUATION WITH INVERSE-POWER POTENTIAL

Shi-Hai Dong[1], **Zhong-Qi Ma**[2,1] and **Giampiero Esposito**[3,4]

[1]*Institute of High Energy Physics, P. O. Box 918(4), Beijing 100039, People's Republic of China*

[2]*China Center for Advanced Science and Technology (World Laboratory), P. O. Box 8730, Beijing 100080*

[3]*INFN, Sezione di Napoli, Mostra d'Oltremare Padiglione 20, 80125 Napoli, Italy*

[4]*Dipartimento di Scienze Fisiche, Complesso Universitario di Monte S. Angelo, Via Cintia, Edificio G, 80126 Napoli, Italy*

The Schrödinger equation for stationary states is studied in a central potential $V(r)$ proportional to $r^{-\beta}$ in an arbitrary number of spatial dimensions. The presence of a single term in the potential makes it impossible to use previous algorithms, which only work for quasi-exactly-solvable problems. Nevertheless, the analysis of the stationary Schrödinger equation in the neighbourhood of the origin and of the point at infinity is found to provide relevant information about the desired solutions for all values of the radial coordinate. The original eigenvalue equation is mapped into a differential equation with milder singularities, and the role played by the particular case $\beta = 4$ is elucidated. In general, whenever the parameter β is even and larger than 4, a recursive algorithm for the evaluation of eigenfunctions is obtained. Eventually, in the particular case of two spatial dimensions, the exact form of the ground-state wave function is obtained for a potential containing a finite number of inverse powers of r, with the associated energy eigenvalue.

Key words: quantum mechanics, scattering states, bound states.

1. INTRODUCTION

Many efforts have been produced in the literature over several decades to study the stationary Schrödinger equation in various dimensions with a central potential containing negative powers of the radial coordinate [1–19]. Some relevant examples are as follows.

(i) When gaseous ions or electrons move through a gas whose molecules are not too large, then the two interact according to the law [3]

$$V(r) = -\frac{1}{2}e^2 \alpha r^{-4}, \tag{1.1}$$

where e is the ionic charge, α the molecular polarizability, and r the distance between the ion and the molecule.

(ii) Interactions in one-electron atoms, muonic and hadronic and Rydberg atoms; photodecay of excited states.

(iii) Repulsive singular potentials, for which the stationary Schrödinger equation has non-Fuchsian singularities at zero and at infinity, may be sometimes expressed by a Laurent series [12–18]

$$V(r) = \sum_{n=-\infty}^{\infty} a_n r^n \tag{1.2}$$

in the annulus $r \in]0, \infty[$.

(iv) The Dirac equation for a spin-$\frac{1}{2}$ particle interacting with scalar, electric and magnetic potentials leads to second-order equations for spinor wave functions involving an effective potential containing terms proportional to r^{-2}, r^{-3} and r^{-4}. Such equations can be used to prove the existence of magnetic resonances between massive and massless spin-$\frac{1}{2}$ particles with magnetic moments [19].

Major progress has been possible when the potential contains a finite number of powers of r, e.g. r^{-1}, r^{-2}, r^{-3} and r^{-4}, or r^2, r^{-4} and r^{-6} [7]. Such a property is not a mathematical accident, because in many cases one only succeeds in finding some eigenstates and eigenvalues for the so-called quasi-exactly-solvable problems [20]. What happens is that an algorithm can be found to evaluate some eigenfunctions provided that a number of coefficients in the potential remain non-vanishing and obey some restrictions, so that enough algebraic equations are obtained for all unknown parameters in the ansatz.

The truly hard mathematical task, however, remains the one of solving the stationary Schrödinger equation with only one term in the potential, or for potentials admitting a Laurent series expansion for $r \in]0, \infty[$. The latter problem is studied by several authors (see [12–18] and references therein) and hence we focus on the former. When the stationary Schrödinger equation is studied for a central potential $U(r)$ in $\mathbf{R}^q$, it reads [18]

$$\left[\frac{d^2}{dr^2} + \frac{(q-1)}{r}\frac{d}{dr} + \kappa - \frac{2m}{\hbar^2}U(r) - \frac{l(l+q-2)}{r^2}\right]\psi(r) = 0, \tag{1.3}$$

where $l(l+q-2)$ results from the action of the Laplace–Beltrami operator on square-integrable functions on the $(q-1)$-sphere. Equation (1.3) can be re-expressed in a form which does not involve first derivatives, i.e. [21]

$$\left[\frac{d^2}{dr^2} + \kappa - V(r) - \frac{(\lambda^2 - \frac{1}{4})}{r^2}\right] y(r) = 0, \tag{1.4}$$

where we have defined [21]

$$\kappa \equiv \frac{2mE}{\hbar^2}, \tag{1.5}$$

$$V(r) \equiv \frac{2m}{\hbar^2}U(r), \tag{1.6}$$

$$\lambda \equiv l + \frac{1}{2}(q-2), \tag{1.7}$$

$$y(r) \equiv r^{\frac{(q-1)}{2}}\psi(r), \tag{1.8}$$

having denoted by m the mass parameter, by E the eigenvalues, by l the angular momentum quantum number and by $\psi(r)$ the radial part of the wave function. The form (1.4) of the stationary Schrödinger equation is the most suitable for applications to scattering problems, because the operator in square brackets is an even function of λ [12, 21].

For a given form of inverse-power potential, Sec. 2 studies the limiting form of Eq. (1.4) as $r \to 0$ and as $r \to \infty$ to obtain a convenient factorization of its solution for all values of r. This involves an unknown function F, and an algorithm for the evaluation of F is developed in Sec. 3, if the inverse power of r in the potential $V(r)$ is even. A class of ground-state wave functions are evaluated in Sec. 4, and concluding remarks are presented in Sec. 5.

2. PROPERTIES OF EIGENFUNCTIONS

For the reasons described in the introduction, we are interested in a potential V having the form (hereafter $\beta > 2$)

$$V(r) \equiv \alpha r^{-\beta}, \tag{2.1}$$

where α and β are some dimensionful and dimensionless parameters, respectively. The first step in the attempt of solving Eq. (1.4) is the search of regular solutions in the neighbourhood of the origin. We therefore look for solutions $y(r)$ taking the limiting form

$$y(r) = r^p e^{-\gamma r^{-\delta}} \text{ as } r \to 0, \tag{2.2}$$

where p, γ and δ are some parameters to be determined by consistency conditions, having taken δ to be positive, as is suggested by known results for some values of β, e.g. when $\beta = 4$. Indeed, on inserting the ansatz (2.2) into Eq. (1.4) one finds when $r \to 0$ the equation (for a fixed value of κ, which is therefore negligible with respect to inverse powers of r)

$$\frac{p(p-1) - (\lambda^2 - \frac{1}{4})}{r^2} + \frac{\gamma\delta(2p-\delta-1)}{r^{\delta+2}} + \frac{\gamma^2\delta^2}{r^{2\delta+2}} - \frac{\alpha}{r^\beta} = 0. \tag{2.3}$$

Since $r \to 0$ and $\delta > 0$, this limiting form of the equation reduces to

$$\frac{\gamma\delta(2p-\delta-1)}{r^{\delta+2}} + \frac{\gamma^2\delta^2}{r^{2\delta+2}} - \frac{\alpha}{r^\beta} = 0. \tag{2.4}$$

Of course, the term proportional to $r^{-2\delta-2}$ dominates over the term proportional to $r^{-\delta-2}$ as $r \to 0$, and hence Eq. (2.4) can only be satisfied if

$$\gamma^2\delta^2 = \alpha, \tag{2.5}$$

$$2\delta + 2 = \beta, \tag{2.6a}$$

which implies that the potential is repulsive (since $\alpha > 0$), and

$$\delta = \frac{\beta}{2} - 1, \tag{2.6b}$$

$$\gamma = \frac{2\sqrt{\alpha}}{(\beta - 2)}. \tag{2.7}$$

So far, p remains undetermined. Note, however, that the coefficient $(2p - \delta - 1)$ in Eq. (2.4) can be taken to vanish. This assumption leads to

$$\delta = 2p - 1, \tag{2.8}$$

and by virtue of (2.6b) and (2.8) one finds $\beta = 4p$. In particular, if $p = 1$, one recovers the familiar limiting form of the solution when the repulsive potential is proportional to r^{-4}:

$$y(r) = re^{-\sqrt{\alpha}r^{-1}} \quad \text{as } r \rightarrow 0. \tag{2.9}$$

In the neighbourhood of the point at infinity, solutions of Eq. (1.4) behave as (hereafter $\varepsilon \equiv \pm 1$)

$$y(r) \sim e^{i\varepsilon r\sqrt{\kappa}} \quad as\ r \rightarrow \infty, \tag{2.10}$$

since only positive values of E are compatible with a repulsive potential. The ansatz for finding solutions of Eq. (1.4) *for all values* of r when the potential (2.1) is considered reads therefore

$$y(r) = e^{-\gamma r^{-\delta}} \ e^{i\varepsilon r\sqrt{\kappa}} F(r), \tag{2.11}$$

where the function F interpolates in between the asymptotic regimes described by (2.2) and (2.10). By virtue of (1.4), (2.1) and (2.11) the function F should solve the differential equation

$$\left[\frac{d^2}{dr^2} + p(r)\frac{d}{dr} + q(r)\right] F(r) = 0, \tag{2.12}$$

where

$$p(r) \equiv 2\gamma\delta r^{-\delta-1} + 2i\varepsilon\sqrt{\kappa}, \tag{2.13}$$

$$q(r) \equiv \gamma^2 \delta^2 r^{-2\delta-2} - \gamma\delta(\delta+1) r^{-\delta-2} + 2i\varepsilon\gamma\delta\sqrt{\kappa} r^{-\delta-1}$$

$$- \alpha r^{-\beta} - \frac{(\lambda^2 - \frac{1}{4})}{r^2}. \tag{2.14}$$

3. ALGORITHM FOR THE EVALUATION OF $F(r)$

If we now assume that (2.5) and (2.6a) remain valid, the formulae (2.13) and (2.14) reduce to

$$p(r) = 2\sqrt{\alpha} r^{-\frac{\beta}{2}} + 2i\varepsilon\sqrt{\kappa}, \tag{3.1}$$

$$q(r) = -\frac{\beta}{2}\sqrt{\alpha} r^{-\frac{\beta}{2}-1} + 2i\varepsilon\sqrt{\alpha\kappa}\, r^{-\frac{\beta}{2}} - \frac{(\lambda^2 - \frac{1}{4})}{r^2}. \tag{3.2}$$

Since we are taking $\beta > 2$, such formulae lead to non-Fuchsian singularities in Eq. (2.12), and hence we look for $F(r)$ in the form

$$F(r) = r^{\omega} \sum_{s=-\infty}^{\infty} a_s r^s \equiv r^{\omega} \sigma(r). \tag{3.3}$$

It is crucial to allow for negative powers of r in the solution, which are associated to the non-Fuchsian nature of the singular point at $r = 0$. By virtue of (2.12) and (3.3), the series σ obeys the second-order equation

$$\left[\frac{d^2}{dr^2} + \left(\frac{2\omega}{r} + p(r)\right)\frac{d}{dr} + \left(\frac{\omega(\omega-1)}{r^2} + \frac{\omega}{r}p(r) + q(r)\right)\right]\sigma(r) = 0. \tag{3.4}$$

In Eq. (3.4), the term $\frac{\omega}{r}p(r) + q(r)$ has the coefficient $\sqrt{\alpha}\left(2\omega - \frac{\beta}{2}\right)$ for $r^{-\frac{\beta}{2}-1}$. We set it to zero to get rid of the dominant singularity at $r = 0$, which implies

$$\omega = \frac{\beta}{4}. \tag{3.5}$$

As a consistency check we point out that, if $\beta = 4$, one recovers the well known value $\omega = 1$ (see (2.9)). For odd values of β, ω is therefore a polydromy parameter for the wave function, as is familiar in singular potential scattering [13,17,18].

If Eq. (3.5) is taken to hold, and if β is even, so that $\frac{\beta}{2}$ is an integer b, Eqs. (3.3) and (3.4) lead to the following recurrence relation among coefficients of the series $\sigma(r)$:

$$
\begin{aligned}
&2\sqrt{\alpha}(s+b+1)a_{s+b+1} + 2i\varepsilon\sqrt{\alpha\kappa}a_{s+b} \\
&+ \left[(s+2)(s+1) + \frac{\beta^2}{16} + \beta\left(\frac{s}{2} - \frac{1}{4}\right) - \left(\lambda^2 - \frac{1}{4}\right)\right] a_{s+2} \\
&+ \left[2i\varepsilon\sqrt{\kappa}(s+1) + \frac{i}{2}\varepsilon\beta\sqrt{\kappa}\right] a_{s+1} = 0, \qquad (3.6)
\end{aligned}
$$

for all integer values of s from $-\infty$ through $+\infty$. Such a formula is even more complicated than the recurrence relation for coefficients of Mathieu functions [22]. Nevertheless, it provides a well defined rule for the evaluation of $F(r)$ for given values of α, when β is even. If β is odd, we no longer get power series, and hence we are unable to obtain a recursive algorithm.

4. A CLASS OF GROUND-STATE WAVE FUNCTIONS

It may be of some interest to conclude our paper by considering a different application of Eq. (1.4), i.e. the evaluation of ground-state wave functions for potentials $V(r)$ containing more than one negative power of r. In such a case an algorithm for bound states, rather than scattering states, can be found provided that the parameters in the potential obey a set of suitable restrictions, and we are now aiming to show how this can be obtained. For simplicity, we set $q = 2$ (bearing also in mind that two-dimensional models are of interest), so that $\lambda = l$ (see (1.7)), and we consider a potential in the form

$$V(r) = \frac{A}{r^4} + \frac{B}{r^3} + \frac{C}{r^2} + \frac{D}{r}. \qquad (4.1)$$

The term $\frac{C}{r^2}$ might indeed be combined with the angular momentum contribution $\frac{(l^2-\frac{1}{4})}{r^2}$, but we prefer to keep them distinct to emphasize their different origin. Our ground-state ansatz for $y(r)$ reads

$$y(r) = \exp k(r), \qquad (4.2)$$

where

$$k(r) \equiv \frac{a}{r} + br + c\log(r) \quad a < 0, \quad b < 0. \tag{4.3}$$

The negative signs of the coefficients a and b are necessary to ensure square integrability at zero and at infinity, respectively. The insertion of the ansatz (4.2) into Eq. (1.4) leads therefore to the equation

$$y''(r) - \left[k''(r) + (k'(r))^2\right] y(r) = 0, \tag{4.4}$$

where the prime denotes the derivative with respect to the variable r. We now express $y''(r)$ from Eq. (1.4) arriving at the equation

$$-E + V(r) - \frac{1}{4r^2} = k''(r) + (k'(r))^2, \tag{4.5}$$

because $l = 0$ in the ground state. The above equations lead therefore to an algebraic equation where we equate coefficients of r^p, for all $p = -4, -3, -2, -1, 0$. Hence we find

$$a^2 = A, \tag{4.6}$$

$$2a(1-c) = B, \tag{4.7}$$

$$c(c-1) - 2ab = C - \frac{1}{4}, \tag{4.8}$$

$$2bc = D, \tag{4.9}$$

$$b^2 = -E. \tag{4.10}$$

This system is solved by

$$a = -\sqrt{A}, \tag{4.11}$$

$$c = 1 - \frac{B}{2a} = 1 + \frac{B}{2\sqrt{A}}, \tag{4.12}$$

$$b = \frac{D}{2c} = \frac{D}{2\left(1 + \frac{B}{2\sqrt{A}}\right)}, \tag{4.13}$$

$$E = -b^2 = -\frac{D^2}{4\left(1 + \frac{B}{2\sqrt{A}}\right)^2}. \tag{4.14}$$

Note that, while (4.11) is consistent with a negative value of a as specified in (4.3), negative values of b are only obtained if $D < 0$ and $c > 0$ or if $D > 0$ and $c < 0$. Moreover, after defining

$$\mu \equiv \frac{B}{2\sqrt{A}}, \tag{4.15}$$

Eq. (4.8) can be expressed in the convenient form

$$C = \frac{1}{4} + \mu(1 + \mu) + \frac{D\sqrt{A}}{(1 + \mu)}. \tag{4.16}$$

For the evaluation of excited states, one has to write the ansatz for $y(r)$ in the form of a product, and the resulting analysis is much harder. For this purpose, a separate paper is in order, which goes beyond the aims of the present work.

5. CONCLUDING REMARKS

The first original result of our paper is given by the formulae (2.11)–(2.14) and (3.1)–(3.6) for the solutions of the stationary Schrödinger equation when a central potential of the form (2.1) is considered in q spatial dimensions, if β is even and larger than 4. If $\beta = 4$, we recover instead the standard result, according to which the regular eigenfunction behaves as $re^{-\sqrt{\alpha}r^{-1}}$ in the neighbourhood of the origin. Although much work had been done in the literature on similar problems [23], an investigation as the one we have proposed was missing to our knowledge.

When the parameter β is odd, or for non-integer values of β larger than 2, the equations of Sec. 2 remain valid, but it is no longer possible to develop a recursive algorithm as we have done in Sec. 3. At the mathematical level, the issue of self-adjoint extensions of our Schrödinger operators deserves careful consideration as well (cf. [24]).

Last, in Sec. 4, the complete form of the ground-state wave function has been obtained in two dimensions when the potential takes the form (4.1). The energy eigenvalue is then given by Eq. (4.14), provided that the conditions (4.11)–(4.13) and (4.16) hold.

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