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Exact Solutions of the Schrödinger Equation with Irregular Singularity

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The 1D nonrelativistic Schrödinger equation possessing an irregular singular point is investigated. We apply a general theorem about existence and structure of solutions of linear ordinary differential equations to the Schrödinger equation and obtain suitable ansatz functions and their asymptotic representations for a large class of singular potentials. Using these ansatz functions, we work out all potentials for which the irregular singularity can be removed and replaced by a regular one. We obtain exact solutions for these potentials and present source code for the computer algebra system Mathematica to compute the solutions. For all cases in which the singularity cannot be weakened, we calculate the most general potential for which the Schrödinger equation is solved by the ansatz functions obtained and develop a method for finding exact solutions.

1. INTRODUCTION

The nonrelativistic Schrödinger equation with singular potentials has been extensively investigated [3, 4, 9, 10, 13, 18–20] in order to obtain exact solutions. Although fast computers provide the calculation of approximate solutions with arbitrary precision, exact solutions can be used to test the efficiency of numerical methods.

There are many applications of singular potentials in atomic, nuclear, and molecular physics: magnetic resonances between massless and massive spin-1/2 particles [2], dipole interaction between two atoms [15], the argon interaction [16], interactions in one-electron atoms, muonic and Rydberg atoms [6], interaction of globular molecules [7], and scattering theory [1, 5, 8, 11, 12, 17, 21].

For a summary of properties of singular potentials see ref. 14.

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In the case of singular potentials $\sim r^{-2}$ around the singular point the Schrödinger equation has solutions of power series type that can be shown to converge at least locally; the Schrödinger equation with a potential of the mentioned type is then said to have a regular singularity. If the potential is singular, but $\sim r^{-k}$, $k > 2$, around the singular point, existence and especially convergence of series solutions are no longer guaranteed; the Schrödinger equation with a potential of this type is then said to have an irregular singularity. Especially in molecular physics there are many applications for such Schrödinger equations.

There are several cases in which the Schrödinger equation with irregular singularity is exactly solved by the use of a certain ansatz function [3, 4, 18, 19]. In most of these cases the ansatz function is given and shown to work correctly, but it is not stated how to find it.

In order to fill this gap, we apply a general theorem about the existence and form of exact solutions of linear ordinary differential equations (ODEs) to the Schrödinger equation (Section 3). We get results on structure and asymptotic expansion of solutions that we use to build ansatz functions. In Section 4 we insert these functions into the Schrödinger equation and calculate special cases in which the irregular singularity can be replaced by a regular one. As a consequence, exact solutions involving power series are available that can be computed by the use of Mathematica programs, which are presented. Section 5 is devoted to the situation that a weakening of the singularity is not possible.

We calculate the most general potential for which the Schrödinger equation is solved by ansatz functions obtained from the existence theorem. We then develop a method to find exact solutions of the Schrödinger equation for a given potential and give an example.

2. PRELIMINARIES

We summarize some definitions from the singularity theory of linear ODEs; see ref. 22 for a comprehensive discussion.

2.1. Classification of Singularities

We call $x = x_0$ a regular singularity of a linear second-order differential equation

$$f''(x) + a(x)f'(x) + b(x)f(x) = 0 \tag{1}$$

if a or b is not analytic at x_0, but the equation can be written in the form

$$x^2 f''(x) + xp(x)f'(x) + q(x)f(x) = 0 \tag{2}$$

with p and q being analytic at x_0.

If (1) cannot be written in the form (2) with p and q analytic at x_0, we call x_0 an irregular singularity of Eq. (1).

We call $r = \infty$ a regular (irregular) singularity of Eq. (1) if $t = 0$ is a regular (irregular) singularity of the equation

$$t^4 g''(t) + \left(2t^3 - t^2 p\left(\frac{1}{t}\right)\right) g'(t) + q\left(\frac{1}{t}\right) g(t) = 0$$

which is derived from Eq. (1) by the change of variables $x = t^{-1}$, $g(t) = f(t^{-1})$.

2.2. Definition of Asymptotic Power Series

Let the function f be defined in an open subset S of the complex plane and having $x = x_0$ as an accumulation point. The power series

$$\sum_{i=0}^{\infty} a_i x^i$$

is said to be an asymptotic power series expansion of f as $x \to x_0$ if

$$\lim_{x \to x_0} x^{-m} \left(f(x) - \sum_{i=0}^{m} a_i x^i \right) = 0 \qquad \forall m \geq 0$$

We then write

$$f(x) \sim \sum_{i=0}^{\infty} a_i x^i, \qquad x \to x_0, \qquad x \in S$$

2.3. The Schrödinger Equation

We investigate the nonrelativistic one-dimensional reduced radial Schrödinger equation given by

$$\phi''(x) + (E - V(x))\phi(x) = 0, \qquad x \geq 0 \tag{3}$$

making the following assumptions:

(a) We use atomic units, that is, $\hbar = 2m = 1$.

(b) The effective potential V can be written in the form

$$V(x) = \sum_{i \in I} v_i x^{-i}$$

with a finite index set I fulfilling $I \subset \mathbb{R}^+$, $\max(I) = h$, and $1 + (h/2) \in I$. The v_i are real-valued numbers. We further assume $v_h > 0$ to guarantee the uniqueness of bound-state energy levels [14]. We take $h > 2$: as can be easily verified from the definition given above, Eq. (3) always possesses an irregular singularity at infinity and additionally in the case $h > 2$ an irregular singularity at zero.

3. APPLICATION OF AN EXISTENCE THEOREM

In this section we apply the following existence theorem to Eq. (3). The theorem and proof can be found, for example, in ref. 23.

Theorem. Let S be an open sector of the complex plane with vertex at the origin and positive central angle not exceeding $\pi/(q+1)$, $q > 1$. Let A be an n by n matrix function holomorphic in S and admitting there an asymptotic power series expansion

$$A(x) \sim \sum_{i=0}^{\infty} A_i x^{-1}, \qquad x \to \infty, \qquad x \in S$$

Assume that all eigenvalues λ_i $(2 \leq i \leq n)$ of A_0 are distinct. Then the differential equation

$$x^{-q} Y'(x) = A(x) Y(x) \tag{4}$$

possesses a fundamental matrix solution of the form

$$Y(x) = \hat{Y}(x) x^D \exp(Q(x)) \tag{5}$$

Here Q is a diagonal matrix whose diagonal elements are polynomials of degree $q+1$. The leading term of Q is

$$\frac{x^{q+1}}{q+1} \operatorname{diag}(\lambda_1, \ldots, \lambda_n)$$

The matrix D is diagonal and constant with respect to x and the matrix $\hat{Y}(x)$ has in S an asymptotic expansion

$$\hat{Y}(x) \sim \sum_{i=0}^{\infty} \hat{Y}_i x^{-i}, \qquad x \to \infty, \qquad x \in S$$

where the leading matrix $\hat{Y}_0$ is nonsingular.

In order to apply the existence theorem to (3), we first write (3) in vectorial form. We get

$$\vec{\phi}\,'(x) = \begin{pmatrix} 0 & 1 \\ V(x) - E & 0 \end{pmatrix} \vec{\phi}(x)$$

By multiplication with x^h the form of the latter equation becomes similar to the form of (4):

$$x^h \vec{\phi}\,'(x) = \begin{pmatrix} 0 & x^h \\ x^h(V(x) - E) & 0 \end{pmatrix} \vec{\phi}(x) \tag{6}$$

Furthermore, all entries of the coefficient matrix are now holomorphic at $x = 0$, since the lowest power occurring in V is given by $-h$.

The existence theorem requires a holomorphic coefficient matrix at $x = \infty$ and a negative power of the independent variable on the left side of (4); to fulfill both conditions we transform (6) by means of

$$x = z^{-1}, \qquad \vec{\psi}(z) = \vec{\phi}(z^{-1}) \tag{7}$$

and get the equation

$$z^{2-h} \vec{\psi}\,'(z) = \begin{pmatrix} 0 & -z^{-h} \\ z^{-h}(E - V(z^{-1})) & 0 \end{pmatrix} \vec{\psi}(z) \tag{8}$$

We see that the coefficient matrix of the latter equation is holomorphic at infinity, so it admits there an asymptotic power series expansion. The leading matrix is given by

$$\lim_{z\to\infty} \begin{pmatrix} 0 & -z^{-h} \\ z^{-h}(E - V(z^{-1})) & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ -v_h & 0 \end{pmatrix}$$

The only eigenvalue of the leading matrix is zero, so we cannot apply the existence theorem to Eq. (8). Instead we have to perform a few transformations on (8) in order to get a coefficient matrix with distinct eigenvalues; the general form of these transformations is given in ref. 23; therefore we do not explain what particular idea is behind each of them.

The first step is to transform (8) in such a way that the leading matrix of the expansion of the coefficient matrix has Jordan canonical form (JCF). To this end, we set

$$\vec{\psi}(z) = \begin{pmatrix} 0 & 1 \\ -v_h & 0 \end{pmatrix} \vec{\Psi}(z) \tag{9}$$

and compute the transformed equation:

$$z^{2-h} \vec{\Psi}\,'(z) = \begin{pmatrix} 0 & (1/v_h) z^{-h}(V(z^{-1}) - E) \\ v_h z^{-h} & 0 \end{pmatrix} \vec{\Psi}(z) \tag{10}$$

Indeed we find that the leading matrix now has JCF:

$$\lim_{z\to\infty} \begin{pmatrix} 0 & (1/v_h) z^{-h}(V(z^{-1}) - E) \\ v_h z^{-h} & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

The latter matrix still has only the eigenvalue zero. To change this, we need two further transformations. The first one guarantees that the transformed leading matrix has the same entry above the main diagonal as the original one has and that it has at least one nonzero entry on or below the main diagonal. The following so-called shearing transformation

$$\vec{\Psi}(z) = \begin{pmatrix} 1 & 0 \\ 0 & z^{-h/2} \end{pmatrix} \vec{\chi}(z) \tag{11}$$

takes Eq. (10) into

$$z^{2-h}\vec{\chi}\,'(z) = \begin{pmatrix} 0 & (1/v_h) z^{-3/2h}(V(z^{-1}) - E) \\ v_h z^{-h/2} & (h/2) z^{1-h} \end{pmatrix} \vec{\chi}(z)$$

Note that the choice of the exponent of z in the shearing transformation is not trivial [23].

Now we perform the last transformation in order to make the leading matrix possess two distinct eigenvalues. We set

$$z = 2^{2/(2-h)} t^2, \qquad \vec{\Phi}(t) = \vec{\chi}(2^{2/(2-h)} t^2) \tag{12}$$

and setting further $\hat{V}(t) = V(2^{-2/(2-h)} t^{-2})$, we arrive at the equation

$$t^{3-h}\vec{\Phi}'(t) = \begin{pmatrix} 0 & (1/v_h) 2^{-2h/(2-h)}(\hat{V}(t) - E) \\ v_h & h t^{2-h} \end{pmatrix} \vec{\Phi}(t) \tag{13}$$

Now the leading matrix is given by

$$\lim_{t \to \infty} \begin{pmatrix} 0 & (1/v_h) 2^{-2h/(2-h)} t^{-2h}(\hat{V}(t) - E) \\ v_h & h t^{2-h} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ v_h & 0 \end{pmatrix} \tag{14}$$

with two distinct eigenvalues $\pm\sqrt{v_h}$.

We are now ready to apply the existence theorem to Eq. (13); let C denote the coefficient matrix of (13).

1. The matrix C is obviously holomorphic, since all entries are. Furthermore, it possesses the following inverse power series expansion that is obtained by inserting the definition of $\hat{V}$ into C:

$$C(t) = \begin{pmatrix} 0 & (1/v_h)^{-2h/(2-h)}\left(t^{-2h}\left(\sum_{i \in I} v_i 2^{2i/(2-h)} t^{2i} - E\right)\right) \\ v_h & h t^{2-h} \end{pmatrix}$$

$$= \begin{pmatrix} 0 & \sum_{i \in I} ((v_i/v_h) 2^{2(i-h)/(2-h)} t^{2(i-h)}) - (1/v_h) 2^{-2h/(2-h)} E T^{-2h} \\ v_h & h t^{2-h} \end{pmatrix}$$

$$= \sum_{i \in I \cup \{0\}} \mathrm{Q}it^{2(i-h)} \tag{15}$$

where

$$C_i = \begin{cases} \begin{pmatrix} 0 & (v_i/v_h)2^{2(i-h)/(2-h)}t^{2(i-h)} \\ 0 & 0 \end{pmatrix} & \text{if} \quad i \in I \backslash \left\{1 + \dfrac{h}{2}\right\} \\ \begin{pmatrix} 0 & -(1/v_h)2^{-2h/(2-h)}Et^{-2h} \\ v_h & 0 \end{pmatrix} & \text{if} \quad i = 0 \\ \begin{pmatrix} 0 & (v_{1+h/2}/v_h)2t^{2-h} \\ 0 & h \end{pmatrix} & \text{if} \quad i = 1 + \dfrac{h}{2} \end{cases}$$

Since $\max(I) = h$, the series (15) is of pure inverse power type. Observe that (15) represents C not only asymptotically, but exactly.

2. By comparison of Eqs. (13) and (4) we see that

$$q = h - 3$$

3. As already seen, the eigenvalues of the leading matrix C_h given in (14) are distinct.

The existence theorem is now applicable. We get existence of a solution of Eq. (13) with the following properties:

1. The solution is defined in any open sector S with central angle less than $\pi/(h - 2)$.

2. The solution is of the form (5), that is,

$$\vec{\Phi}(t) = \vec{\hat{\Phi}}(t)\, t^D \exp(Q(t)) \tag{16}$$

where

$$\vec{\hat{\Phi}}(t) \sim \sum_{i=0}^{\infty} \vec{\varphi}_i t^{-i}, \qquad t \to \infty, \qquad t \in S$$

$$D = \mathrm{diag}(d_1, d_2) \tag{17}$$

$$Q(t) = \mathrm{diag}\left(\sum_{i=0}^{h-3} a_i t^{-i} + \frac{\sqrt{v_h}t^{h-2}}{h-2}, \sum_{i=0}^{h-3} b_i\, t^{-i} - \frac{\sqrt{v_h}\, t^{h-2}}{h-2}\right)$$

Using these settings, we can specify t^D and $\exp(Q(t))$:

$$t^D = \mathrm{diag}\,(t^{d_1}, t^{d_2})$$

$$\exp(Q(t)) = \mathrm{diag}\left(\exp\left(\sum_{i=0}^{h-3} a_i t^{-i} + \frac{\sqrt{v_h}t^{h-2}}{h-2}\right), \exp\left(\sum_{i=0}^{h-3} b_i t^{-i} - \frac{\sqrt{v_h}t^{h-2}}{h-2}\right)\right).$$

Since we now know the structure of solutions of (13), we want to get from (16) an ansatz for solutions of the original equation (3). To this end, we have to transform the function $\vec{\Phi}$ back into $\vec{\phi}$, that is, we have to apply the inverse of all transformations performed above on $\vec{\Phi}$. More explicitly, we have to do the following:

1. Inverse coordinate transformation (12):

$$t = \sqrt{2^{2/(h-2)}}z, \qquad \vec{\chi}(z) = \vec{\Phi}\,(\sqrt{2^{2/(h-2)}}z)$$

2. Inverse shearing transformation (11) and inverse transformation (9):

$$\vec{\psi}(z) = \begin{pmatrix} 0 & 1 \\ -v_h & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & z^{-h/2} \end{pmatrix} \vec{\chi}(z)$$

3. Inverse coordinate transformation (7):

$$z = x^{-1}, \qquad \vec{\phi}(x) = \vec{\psi}(x^{-1})$$

Doing these transformations, we obtain the following expression for $\vec{\phi}$:

$$\vec{\phi}(x) = \vec{\hat{\Phi}}(2^{1/(h-2)}x^{-1/2}) \times \left[2^{d_2/(h-2)} \exp\left(\sum_{i=0}^{h-3} b_i(2^{i/(h-2)}x^{-i/2}) - \frac{2x^{(2-h)/2}\sqrt{v_h}}{h-2} \right) x^{(h-d_2)/2}, \right.$$
$$\left. v_h 2^{d_1/(h-2)} \exp\left(\sum_{i=0}^{h-3} a_i(2^{i/(h-2)}x^{-i/2}) + \frac{2x^{(2-h)/2}\sqrt{v_h}}{h-2} \right) x^{-d_1/2} \right] \quad (18)$$

where $\vec{\hat{\Phi}}$ possesses an asymptotic expansion of the form

$$\vec{\hat{\Phi}}(x) \sim \sum_{i=0}^{\infty} \vec{\varphi}_i 2^{i/(2-h)} x^{i/2}, \qquad x \to 0 \quad (19)$$

valid in the transformed set $\hat{S} = 2^{1/(h-2)}\, S^{-1/2}$, where S denotes the sector in which (17) holds.

For completeness let us briefly describe the shape of $\hat{S}$. Using polar coordinates we find for $x = R_x \exp(i\varphi_x) \in S$ and integer k

$$2^{1/(h-2)}\, z^{-1/2} = 2^{1/h-2}\, (R_x \exp\,(i(\varphi_x + 2k\pi)))^{-1/2}$$
$$= 2^{1/h-2} R_x^{-1/2} \exp\left(i\left(-\frac{\varphi}{2} - k\pi \right)\right)$$

meaning that

$$(0, \infty) \ni R_x \mapsto R_x^{-1/2} \in (0, \infty)$$

$$\left(0, \frac{\pi}{h-2}\right) \ni \varphi_x \mapsto \begin{cases} -\frac{\varphi_x}{2} \in \left(-\frac{\pi}{2h-4}, 0\right) & \text{if} \quad k = 0 + 2\mathbb{N}_0 \\ -\frac{\varphi_x}{2} - \pi \in \left(-\pi, -\frac{\pi(2h-3)}{2h-4}\right) & \text{if} \quad k = 1 + 2\mathbb{N}_0 \end{cases}$$

that is, the sector S loses one half of its original angle and is mirrored at the real axis and rotated by π (only if $k = 1$).

4. REDUCTION TO REGULAR SINGULARITY CASE

Since by (18) we know the structure of solutions of (3), we can build ansatz functions possessing that structure. We insert the first component of (18) as an ansatz function into the Schrödinger equation (3) and have to determine the unknown function $\vec{\hat{\Phi}}$. At first we do not make use of the known asymptotic expansion (19), but assume $\vec{\hat{\Phi}}$ to be completely unknown. Denoting the first component of $\vec{\hat{\Phi}}$ by $\hat{\Phi}$, d_2 by d, inserting the first component of (18) into (3), and collecting terms, we obtain the following equation for $\hat{\Phi}$:

$$\begin{aligned}
&\hat{\Phi}''(x)x^2 \\
&\quad + \hat{\Phi}'(x)x\Bigg(x^{3/2}\left(2^{1/(h-2)}3 + 2^{1-1/(h-2)}d - 2^{1-1/(h-2)}h\right) \\
&\quad + x^{5/2}2^{2-1/(h-2)}\left(\sum_{i=0}^{h-3}\frac{ih_i}{2}2^{2i/(2h-4)}x^{-i/2-1}\right) - x^{(5-h)/2}2^{1-(h+3)/(h-2)}\sqrt{v_h}\Bigg) \\
&\quad + \hat{\Phi}(x)(x^3(2^{1-2/(h-2)}d + d^2 2^{2/(2-h)} - 2^{1-2/(h-2)}h - 2^{1-2/(h-2)}dh + h^2 2^{2/(2-h)}) \\
&\quad + x^4\Bigg(2^{2-2/(h-2)}(d-h)\left(\sum_{i=0}^{h-3}\frac{ih_i}{2}2^{2i/(2h-4)}x^{-i/2-1}\right) \\
&\quad - 2^{1-h+4/(h-2)}d\sqrt{v_h}x^{-h/2} + 2^{h-4/(h-2)}h\sqrt{v_h}x^{-h/2}\Bigg) \\
&\quad + x^5\Bigg(2^{2-2/(h-2)}(E - V(x) + 1)\left(\sum_{i=0}^{h-3}\frac{b_i}{2}2^{2i/(2h-4)}(-i)\left(-\frac{i}{2} - 1\right)x^{-i/2-2}\right) \\
&\quad + 2^{2-2/(h-2)}\left(\sum_{i=0}^{h-3}\frac{ib_i}{2}2^{2i/(2h-4)}x^{-(i/2)-1}\right)^2 \\
&\quad - 2^{2-(h+4)/(h-2)}\left(\sum_{i=0}^{h-3}\frac{ih_i}{2}2^{2i/(2h-4)}x^{-i/2-1}\right)\sqrt{v_h}x^{-b/2} + (2^{-6/(h-2)+2h/(h-2)}v_h)x^{-h}\Bigg) = 0
\end{aligned}$$

Our aim is to find potential V and parameters $h > 2$, d, and c_i such that $x = 0$ is a regular singularity for the latter equation. We then know that there are solutions for $\hat{\Phi}$ admitting locally convergent series expansions [23]. First we restrict consideration to the case $h = 3$, meaning that all sums in (20) running to $h - 3$ contain only one term.

4.1. The Case $h = 3$

According to Section 2, the lowest power occurring in the potential V is given by $-h = -3$. Simplifying Eq. (20) by setting $h = 3$ yields the equation

$$x^2\hat{\Phi}''(x) + \left(\left(d - \frac{3}{2}\right)x^{3/2} - 2x\sqrt{v_3}\right)x\hat{\Phi}'(x) + \left(\left(\frac{3}{4} - d + \frac{d^2}{4}\right)x^3 + (E - V(x))x^5 + x^{5/2}\sqrt{v_3}\left(\frac{3}{2} - d\right) + x^2 v_3\right)\hat{\Phi}(x) = 0 \tag{20}$$

For zero being a regular singular point, we require the bracketed parts of the coefficients of $\hat{\Phi}'$ and $\hat{\Phi}$ to be analytic, meaning that the roots have to be removed. This is done by choosing $d = 3/2$, which leads to the equation

$$x^2\hat{\Phi}''(x) - (2x\sqrt{v_3})x\hat{\Phi}'(x) + \left(-\frac{3}{16}x^3 + (E - V(x))x^5 + x^2 v_3\right)\hat{\Phi}(x) = 0 \tag{21}$$

We see that the latter equation has zero as a regular singular point provided the potential V does not involve nonanalytic terms, which we assume in what follows.

We infer that (21) possesses solutions of the form

$$\hat{\Phi}(x) = \sum_{i=0}^{\infty} c_i x^{i+s} \tag{22}$$

where the exponents at the regular singularity zero are determined by the indicial equation, which reads

$$s(s - 1) = 0$$

The exponents are thus given by

$$s = 0, \qquad s = 1$$

Taking the larger one, we set $s = 1$ and insert the power series (22) into Eq.

(21). We are now ready to obtain the expansion coefficients c_i by computing a recurrence formula for the c_i in the usual way. Since calculating of a few of these coefficients and presenting them here does not lead to new insights, we instead give the source of a computer program for Mathematica that performs the required calculations (see Fig. 1).

Description of the Program. We name the input and output variables used in the program; the rest is obvious.

Input:
• $f[x]$: The function $\hat{\Phi}$ to calculate; this should not be changed.
• p: Desired expansion order of $\hat{\Phi}$; may be changed.

```
Clear["`*"];

p = 10;
f[x_] := Sum[c[i]*x^(i + 1), {i, 0, p+3}];
pot = Sum[v[i]/x^i, {i, 1, 3}];

eq = Expand[f[x]*(-3*x^3/16 + (e - pot)*
            x^5 + x^2*v[3]) -
            2*x^2*Sqrt[v[3]]*D[f[x], x] +
            x^2*D[f[x], {x, 2}]];

ps[0] = Solve[Coefficient[eq, x^2] == 0,
              c[1]][[1,1,2]];
For[i = 1, i <= p, i++,
    ps[i] = Solve[Coefficient[eq,
                  x^(2 + i)] == 0,
                  c[i + 1]][[1,1,2]];
    For[j = 1, j <= i, j++,
        ps[i] = ps[i] /. c[j] -> ps[j - 1];];
    ];

solution = Expand[Collect[Sum[ps[i]*x^(i + 1),
           {i, 0, p}], x]];
```

Fig. 1. Computer program for calculating $\hat{\Phi}$ for the case $h = 3$.

• *pot*: The potential V; may be changed, but should not contain nonanalytic terms.

• *eq*: Eq. (21); should not be changed.

Output:

• *solution*: The function $\hat{\Phi}$, expanded up to order p.

• *ps*[*i*]: The expansion coefficients of $\hat{\Phi}$, depending only on the first of them, *ps*[0]; The index i runs from 0 to p.

A generalization. There is a generalization of the results obtained in the previous paragraph. Until now we have assumed that V is of the form given in Section 2 with lowest power $-h = -3$. Now we drop this assumption. We then see that the coefficient of $\hat{\Phi}$ in (21) is analytic at zero even if V contains terms $\sim x^{-5}$. In particular, there are solutions of (21) of the form (22) if $V(x)x^5$ is analytic at zero.

To obtain these solutions, one has to insert the ansatz (22) into Eq. (21). Note that the indicial equation and the exponents may change; for example, picking the inverse power potential

$$V(x) = \sum_{i=0}^{5} v_i x^{-i}$$

one is led to the indicial equation

$$s^2 - s - v_5 = 0$$

with solutions

$$s = \frac{1}{2}(1 + \sqrt{1 + 4v_5})$$

Taking the larger one, that is, $s = \frac{1}{2}(1 + \sqrt{1 + 4v_5})$, we can use the modified version of the above program to compute the solutions (see Fig. 2). The inputs and outputs of the program are the same as of the first one.

4.2. The Case $h > 3$

We return to the general equation (20); in particular, we examine the bracketed coefficients of $\hat{\Phi}$ and $\hat{\Phi}'$ in order to find out how to choose the free parameters to convert the irregular singularity at zero into a regular one if $h > 3$.

From (20), in particular from the coefficient of $\hat{\Phi}'$, we see that we need analyticity at zero of the expression

```
Clear["`*"];

p = 10;
f[x_] := Sum[c[i]*x^(i + 1/2*(1 + Sqrt[1 +
            4*v[5]])),
        {i, 0, p + 3}];
pot = Sum[v[i]/x^i, {i, 1, 5}];

eq = Expand[f[x]*(-3*x^3/16 + (e - pot)*
            x^5 + x^2*v[3]) -
            2*x^2*Sqrt[v[3]]*D[f[x], x] +
            x^2*D[f[x], {x, 2}]];

ps[0] =
    Solve[Coefficient[Expand[x^(1/2)*
          eq/x^(1/2*Sqrt[1+4*v[5]])],
          x^2] == 0, c[1]][[1,1,2]];
For[i = 1, i <= p, i++,
    ps[i] =
    Solve[Coefficient[Expand[x^(1/2)*
          eq/x^(1/2*Sqrt[1+4*v[5]])],
          x^(2 + i)] == 0, c[i + 1]]
          [[1,1,2]];
    For[j = 1, j <= i, j++, ps[i] =
        ps[i] /. c[j] -> ps[j - 1];];
    ];

solution = Expand[Collect[Sum[ps[i]*x^(i +
                  1/2*(1 + Sqrt[1 +
                  4*v[5]])), {i, 0, p}], x]];
```

Fig. 2. Computer program for calculating $\hat{\Phi}$ for the case $h = 3$ for a more general potential.

$$x^{3/2}(2^{1/(h-2)}3 + 2^{1-1/(h-2)}d - 2^{1-1/(h-2)}h)$$
$$+ x^{5/2}2^{2-1/(h-2)}\left(\sum_{i=0}^{h-3} \frac{ib_i}{2} 2^{2i/(2h-4)}x^{-i/2-1}\right) - x^{5-h/2}2^{1+(h-3)/(h-2)}\sqrt{v_h} \quad (23)$$

The latter expression contains the following powers of x:

$$\frac{3}{2}, \quad \frac{5-h}{2}, \quad \frac{3-i}{2} \qquad (0 \leq i \leq h-3) \qquad (24)$$

The set of powers given by the third expression in (24) reads explicitly

$$\frac{3-i}{2} \in \left\{1, \frac{1}{2}, 0, -\frac{1}{2}, -1, \ldots, \frac{6-h}{2}\right\} \qquad (25)$$

where the power belonging to $i = 0$ vanishes due to the i contained in the expansion coefficient [see (23)].

The powers given by the expressions in (24) are distinct:

$$\frac{5-h}{2} \overset{?}{=} \frac{3-i}{2} \Rightarrow i = h-2$$

which is impossible, since $i \leq h - 3$. Furthermore, the coefficient of $x^{3/2}$ has to vanish, that is,

$$2^{1/(h-2)}\, 3 + 2^{1-1/(h-2)}\, d - 2^{1-1/(h-2)}\, h = 0 \Rightarrow d = h - \frac{3}{2}$$

So we have to require

$$\frac{5-h}{2} \in \mathbb{N}_0 \Rightarrow h = 5$$

In the case $h = 5$ and $d = h - \frac{3}{2} = \frac{7}{2}$, expression (23) simplifies to

$$2b_1x + 4b_2 2^{1/3}x^{1/2} - 2\sqrt{v_5}2^{2/3}$$

and clearly we have to set

$$b_2 = 0$$

Using these settings, we simplify the coefficient of $\hat{\Phi}$ in (20):

$$-\frac{3}{2^{2/3+2}}x^3 + 2^{1/3+1}(E - V(x))x^5 + b_1{}^2x^2 - 2^{1/3+1}\sqrt{v_5}x^{3/2}$$
$$- 2^{2/3+1}b_1\sqrt{v_5}x + 2^{1/3+1}v_5$$

The only nonanalytic term contained in the latter expression is $x^{3/2}$ provided the potential contributes only analytic terms. Since the coefficient of $x^{3/2}$ never vanishes, we have to require the potential to contain a term $\sim x^{-7/2}$ (note that we needed this condition already in a more general context: in Section 2.3 we assumed the index set I to contain the number $1 + b/2$.) We then get the following relation:

$$v_{7/2} + \sqrt{v_5} = 0$$

Altogether we get that all potentials V possessing the form

$$V(x) = -\sqrt{v_5}\, x^{-7/2} + \hat{V}(x)$$

where $\hat{V}(x)x^5$ is analytic at zero, admit exact solutions of (20) that are of the form (22). To obtain these solutions, as in the case $h = 3$, we insert the ansatz (22) into Eq. (20), which now reads

$$\begin{aligned} & x^2\hat{\Phi}''(x) + (2b_1x - 2\sqrt{v_5}2^{2/3})x\hat{\Phi}'(x) \\ & + \left(-\frac{3}{2^{2/3+2}}x^3 + 2^{1/3+1}(E - V(x))x^5 \right. \\ & \left. + b_1{}^2x^2 - 2^{2/3+1}b_1\sqrt{v_5}x + 2^{1/3+1}v_5\right)\hat{\Phi} = 0 \end{aligned}$$

The indicial equation is given by

$$s(s - 1 - 2^{2/3+1}\sqrt{v_5}) = 0$$

with solutions

$$s = 0, \qquad s = 1 + 2^{2/3+1}\sqrt{v_5}$$

Figure 3 shows a computer program that calculates $\hat{\Phi}$; the inputs and outputs are mostly the same as in the case $h = 3$, (see Figs. 1 and 2).

There are no more cases left in which the irregular singularity at zero can be transformed into a regular one.

5. ANALYSIS OF THE GENERAL POTENTIAL

If the irregular singularity can not be weakened, it does not make sense to insert an ansatz of power series type into (20) in order to obtain solutions. Instead, we solve (20) for the shifted potential $V - E$ and solve the most general potential equation (20) by the ansatz functions built from the existence theorem. This general potential is given in terms of $\hat{\Phi}$, its derivatives, and a few parameters. The problem to solve is: Given a certain potential that is a special case of the general potential, what is the correct choice of $\hat{\Phi}$ and the parameters to reduce the general potential to the special case?

```
Clear["`*"];

p = 10;
f[x_] := Sum[c[i]*x^(i + 1 + 2^(2/3 +
            1)*Sqrt[v[5]]),
           {i, 0, p + 3}];
pot = Sum[v[i]/x^i, {i, 1, 5}] -
          Sqrt[v[5]]/x^(7/2);

eq = Expand[f[x]*(-((3*x^3)/(4*
           2^(2/3))) + (2*2^(1/3)*e -
           2*2^(1/3)*pot)*x^5 + x^2*
           b[1]^2 - x^(3/2)*2*2^(1/3)*
           Sqrt[v[5]]-x*2*2^(2/3)*
           b[1]*Sqrt[v[5]] + 2*
           2^(1/3)*v[5]) + (2*x^2*
           b[1] - 2*2^(2/3)*x*
           Sqrt[v[5]])*D[f[x],x] +
           x^2*D[f[x],{x,2}]];

ps[0] = Solve[Coefficient[eq/x^(2*
             2^(2/3)*Sqrt[v[5]]),
             x^2] == 0,
             c[1]][[1,1,2]];
For[i = 1, i <= p, i++, ps[i] =
    Solve[
    Coefficient[
    Expand[eq/x^(2*2^(2/3)*
           Sqrt[v[5]])], x^(2 + i)] == 0,
           c[i + 1]][[1,1,2]];
    For[j = 1, j <= i, j++, ps[i] =
        ps[i] /. c[j] -> ps[j - 1]; ];
   ];
solution=Expand[
         Collect[
         Sum[ps[i]*x^(i+1),{i,0,p}],x]];
```

Fig. 3. Computer program for calculating $\hat{\Phi}$ for the case $h = 5$.

As one can see from (20), the expression for the general potential is rather lengthy and is given by

$$
\begin{aligned}
V(x) - E = {} & 4^{(1+h)/(2-h)} x^{-9/(2-h)} (2^{(4+h)/(h-2)}\, dx^{5/2+h} \\
& + 64^{1/(h-2)}\, d^2 x^{5/2+h} - 2^{(4+h)/(h-2)}\, hx^{5/2+h} \\
& - 2^{(4+h)/(h-2)}\, dhx^{5/2+h} + 64^{1/(h-2)}\, h^2 x^{5/2+h} \\
& + 2^{2(1+h)/(h-2)} x^{9/2+h} \sum_{i=0}^{h-3} b_i \left(-\frac{i}{2}\right) \\
& \times \left(-\frac{i}{2} - 1\right) 2^{2i/(2h-4)} x^{-i/2-2} + 2^{2(1+h)/(h-2)} x^{9/2+h} \left(\sum_{i=0}^{h-3} b_i \left(-\frac{i}{2}\, 2^{2i/(2h-4)} \right.\right. \\
& \left.\left. \times\, x^{-i/2-1}\right)\right)^2 + \left(\sum_{i=0}^{h-3} b_i \left(-\frac{i}{2}\, 2^{2i/(2h-4)} x^{-i/2-1}\right)\right) (2^{2(1+h)/(h-2)} (h - d) \\
& \left. \times\, x^{7/2+h} + 8^{h/(h-2)} x^{9+h/2} \sqrt{v_h}\right) - 2^{2(1+h)/(h-2)}\, dx^{7+h/2} \sqrt{v_h} + 2^{(4+h)/(h-2)} h \\
& \left. \times\, x^{7+h/2} \sqrt{v_h} + 2^{2(1+h)/(h-2)} x^{9/2} v_h \right) \\
& + \frac{\hat{\Phi}'(x)}{\hat{\Phi}(x)} \left(4^{h/(2-h)} x^{-9/2-h} \left((3 \cdot 32^{1/(h-2)} + 2^{(3+h)/(h-2)} (d - h)) x^{2+h} \right.\right. \\
& \left.\left. + 2^{2+5/(h-2)} x^{3+h} \sum_{i=0}^{h-3} b_i \left(-\frac{i}{2}\right) 2^{2i/(2h-4)} x^{-i/2-1} - 2^{(2h+1)/(h-2)} x^{6+h/2} \sqrt{v_h} \right)\right) \\
& + \frac{\hat{\Phi}''(x)}{\hat{\Phi}(x)} \left(\frac{2^{-2+2/(h-2)}}{x^3} \right)
\end{aligned} \tag{26}
$$

We see that the latter expression splits into three parts: the first part contains only terms independent of $\hat{\Phi}$, the second part depends on $\hat{\Phi}'/\hat{\Phi}$, and the third part depends on $\hat{\Phi}''/\hat{\Phi}$. Due to the length of (26) it does not make sense to analyze it without some knowledge of $\hat{\Phi}$. So we will work out strategies for choosing $\hat{\Phi}$ in order to obtain from (26) a particular type of potential.

To this end, let us analyze the first part, which contains the following negative powers of x:

$$-2, \quad -\frac{i}{2} - 2 \quad (0 \leq i \leq h - 3), \qquad -\frac{i}{2} - 2 \quad (0 \leq i \leq 2h - 6)$$

$$-\frac{h}{2} - 1, \quad -\frac{i+h}{2} - 1 \quad (0 \leq i \leq h-3), \qquad -h$$

All these powers are negative, so the simplest choice $\hat{\Phi}(x) = \text{const}$ is not possible since parts two and three of (26) then vanish, but we need a constant term in (26) due to $E \neq 0$.

The calculation of $\hat{\Phi}$ can be done in the following simple way. According to the potential one wants to construct from (26), one requires the second part of (26) to equal a certain function, say q. Denote by p the coefficient of $\hat{\Phi}'(x)/\hat{\Phi}(x)$ in the second part of (26); then the condition reads

$$\begin{aligned} p(x)\,\frac{\hat{\Phi}'(x)}{\Phi(x)} &\stackrel{!}{=} q(x) \\ \Rightarrow \frac{\hat{\Phi}'(x)}{\hat{\Phi}(x)} &= \frac{q(x)}{p(x)} \\ \Rightarrow \hat{\Phi}(x) &= \exp\left(\int \frac{q(x)}{p(x)}\,dx\right) \end{aligned} \tag{27}$$

If the function q is not too complicated or transcendent, the latter integral can be computed symbolically. If a direct symbolical calculation is not possible, one should expand the expression a/p into a power series which clearly is symbolically integrable. Observe that a numerical computation of the integral is always possible, but in this context senseless, since the parameters $b_1, d, \ldots$ are not known and cannot be set to certain values without determining the whole potential.

Now assume that $\hat{\Phi}$ solves (27). The third part of (26) then contributes the following:

$$\begin{aligned} \frac{\hat{\Phi}''(x)}{\hat{\Phi}(x)}\left(\frac{2^{-2+2/h-2}}{x^3}\right) = &\left(\left(\frac{q(x)}{p(x)}\right)^2\right. \\ &\left. + \frac{q'(x)p(x) - q(x)p'(x)}{p^2(x)}\right)\left(\frac{2^{-2+2/(h-2)}}{x^3}\right) \end{aligned} \tag{28}$$

Altogether we have obtained the following: The function $\hat{\Phi}$ as given in (27) solves Eq. (20) for the shifted potential

$$\begin{aligned} V(x) - E = {} & r(x) + q(x) \\ & + \left(\left(\frac{q(x)}{p(x)}\right)^2 + \frac{q'(x)p(x) - q(x)p'(x)}{p^2(x)}\right)\left(\frac{2^{-2+2/(h-2)}}{x^3}\right) \end{aligned}$$

where r denotes the first part of (26), q is an arbitrary function, and p is the coefficient of $\hat{\Phi}'/\hat{\Phi}$ (26). Observe that either q or the third term in the latter expression must involve a constant term that can be identified with $-E$.

Example. We consider the case $h = 7$, $b_i = 0$ $(1 \le i \le 4)$. The constants b_i are set to zero because otherwise the expressions involved become too long to be included here. The potential (26) then simplifies to

$$V(x) - E = \frac{35/4 - 3d + d^2/4}{x^2} + \frac{\sqrt{v_7}(7/2 - d)}{x^{9/2}} + \frac{v_7}{x^7} + \frac{\hat{\Phi}'(x)}{\hat{\Phi}(x)}\left(\frac{2^{-11/(4/5+1)} + d \cdot 2^{-4/5}}{x^{5/2}}\right) + \frac{\hat{\Phi}''(x)}{\hat{\Phi}(x)2^{3/5+1}x^3} \tag{29}$$

Now we require the second part, that is, the coefficient of $\hat{\Phi}'/\hat{\Phi}$, to equal a constant C that is identified with the energy E. Using the notation defined above, we now have

$$q(x) = C$$

$$p(x) = 2^{-11/(4/5+1)} + \frac{d \cdot 2^{-4/5}}{x^{5/2}}$$

According to formula (27), we obtain after simplification

$$\hat{\Phi}(t) = \exp\left(\int \frac{2^{4/5+1}Cx^5}{(-11 + 2d)x^{5/2} - 4\sqrt{v_7}}\, dx\right) \tag{30}$$

The latter integral can symbolically be found, for example, using Mathematica or any other computer algebra system; unfortunately, the result is definitely too large to be displayed here. As explained above, we can use a power series expansion. We expand the second part of the potential (29) into a power series about zero. This yields

$$\frac{2^{4/5+1}Cx^5}{(-11 + 2d)x^{5/2} - 4\sqrt{v_7}} = -\sum_{i=0}^{\infty} \frac{C(2d - 11)^i}{4^i 2^{1/5} v_7^{(i+1)/2}}\, x^{(10+5i)/2}$$

Inserting the latter expression into the integral, we can compute the solution:

$$\begin{aligned}\hat{\Phi}(x) &= \exp\left(-\int \sum_{i=0}^{\infty} \frac{C(2d - 11)^i}{4^i 2^{1/5} v_7^{(i+1)/2}}\, x^{(10+5i)/2}\, dx\right) \\ &= \exp\left(-\sum_{i=0}^{\infty} \frac{C(2d - 11)^i}{4^i 2^{1/5} v_7^{(i+1)/2}} \int x^{(10+5i)/2}\, dx\right) \\ &= \exp\left(-\sum_{i=0}^{\infty} \frac{C(2d - 11)^i (12 + 5i)}{4^i 2^{1/5} v_7^{(i+1)/2}(10 + 5i)}\, x^{(12+5i)/2}\right)\end{aligned} \tag{31}$$

Observe that the factor $2^{-1/5}$ corresponds to the factor $2^{i/(2-h)}$ contained in the asymptotic expansion (19): Expansion of (31) into a Taylor series at zero generates terms $\sim 2^{i/(2-h)} = 2^{-i/5}$.

The third part of (29), given by (28), simplifies to

$$\left(\frac{C^2}{p^2(x)} - \frac{Cp'(x)}{p^2(x)}\right)\left(\frac{2^{-8/5}}{x^2}\right)$$

that is, more explicitly,

$$\frac{Cx(5\cdot 2^{1/5}(-11 + 2d)\, x^{5/2} + 8\, Cx^6 - 40 \cdot 2^{1/5}\sqrt{v_7})}{2((-11 + 2d)x^{5/2} - 4\sqrt{v_7})^2} \tag{32}$$

Altogether we have found that if $\hat{\Phi}$ is given by (30), respectively (31), then it solves Eq. (20) for the shifted potential

$$V(x) - E = \frac{35/4 - 3d + d^2/4}{x^2} + \frac{\sqrt{v_7}(7/2 - d)}{x^{9/2}} + \frac{v_7}{x^7} + C + \frac{Cx(5 \cdot 2^{1/5}(-11 + 2d)x^{5/2} + 8Cx^6 - 40 \cdot 2^{1/5}\sqrt{v_7})}{2((-11 + 2d)x^{5/2} - 4\sqrt{v_7})^2}$$

Energy eigenvalues are obtained by conditions on the third part of the latter potential.

A natural way of using the described method is the following. Given a certain potential, one chooses a function q and calculates the contribution of the third part of (26), given by (28); observe that knowledge about $\hat{\Phi}$ is not necessary to do this. If the terms (28) are not suitable, one chooses another q and so on, until (28) is acceptable. Then one tries to find $\hat{\Phi}$ by direct integration; see (27). If this fails, one expands q/p into a power series and thereafter uses integration. If no closed expression as in the example can be found, at least expansion up to arbitrary order is possible.

Clearly all calculations should be carried out using a computer algebra system.

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