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A FORMAL SERIES SOLUTION OF THE ONE-DIMENSIONAL SCHRÖDINGER EQUATION

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Abstract. An asymptotic expansion of the solution y of the initial value problem to the one-dimensional Schrödinger equation $y'' + uy = 0$ is derived. If the potential u is analytic or if the expansion has only finitely many terms then the formal series represents an effective solution.

Key words. One-dimensional Schrödinger equation, initial-value problem, asymptotic expansion, formal solution.

MS classification. 34 A 30, 34 A 05.

INTRODUCTION

Let us consider the one-dimensional Schrödinger operator, sometimes also called Sturm-Liouville operator,

$$L := \frac{d^2}{dx^2} + u, \tag{1}$$

with a smooth potential $u = u(x)$. (Here and in the following smooth means C^∞.) We associate to the initial-value problem

$$\begin{gathered} Ly = y'' + uy = 0, \\ y(x_0) = y_0, \qquad y'(x_0) = y'_0 \end{gathered} \tag{2}$$

the sequence of two-point functions $Y_n = Y_n(x, x_0)$ $(n = 0, 1, 2, \dots)$ which is uniquely defined by the recursion

$$\begin{gathered} 2(x - x_0)\, n \frac{\partial}{\partial x} Y_n + n(n-1)\, Y_n + LY_{n-2} = 0 \qquad \text{for } n \geq 2, \\ Y_0 := y_0, \qquad Y_1 := y'_0. \end{gathered} \tag{3}$$

The main result is that the solution of (2) admits the asymptotic expansion

$$y \sim \sum_{n=0}^{\infty} Y_n \cdot (x - x_0)^n \qquad \text{for } x \to x_0. \tag{4}$$

The formal series on the right-hand side of (4) turns into an effective solution of (2) if $u = u(x)$ is an analytic function or if the sequence $Y_n = Y_n(x, x_0)$ breaks off (that means, reduces to zero) after a finite number of terms. We will demonstrate both these possibilities by examples.

The idea for (4) has been to find a one-dimensional analog of J. Hadamard's classical construction of an elementary solution to a second-order linear partial differential equation [3]. J. E. Lagnese [5] used such an analogy for writing down a distributional fundamental solution to L. We will work here with functions, not with distributions. The quantities Y_{2m+1} with an odd index $2m + 1$ are directly analogous to Hadamard's coefficients U_m, while the quantities Y_{2m} with an even index $2m$ are introduced here for the first time. The author has reviewed in the papers [6, 7] the relevance of the sequence Y_{2m+1} $(m = 0, 1, 2, \ldots)$ for spectral theory and Huygens' principle. Moreover, the diagonal values $Y_{2m+1}(x, x)$ have to do with the Korteweg-de Vries hierarchy of solitonic partial differential equations [6, 7].

DERIVATION OF THE ASYMPTOTIC EXPANSION

A linear differential operator of the form

$$D_n := 2(x - x_0)\frac{\mathrm{d}}{\mathrm{d}x} + n \qquad \text{with } n > 0, \tag{5}$$

acting on functions of x which are smooth in the vicinity of x_0, has a unique inverse D_n^{-1}. More precisely, there holds.

Proposition 1. Let $f = f(x)$ be defined and smooth in some open interval containing x_0 and $n > 0$. Then $D_n y = f$ has a unique smooth solution $y = y(x)$ in *dom f*, given by

$$2y(x) = \int_0^1 \lambda^{n/2-1} f(\lambda x + (1 - \lambda)\, x_0)\, \mathrm{d}\lambda. \tag{6}$$

(Here and in the following *dom* means domain of definition.)

Proof. For $n \geq 2$ we verify

$$D_n y = \int_0^1 \left[\lambda^{n/2}(x - x_0)\, f' + \frac{n}{2}\lambda^{n/2-1} f\right] \mathrm{d}\lambda =$$
$$= \int_0^1 \frac{\mathrm{d}}{\mathrm{d}\lambda}[\lambda^{n/2} f]\, \mathrm{d}\lambda = f(x),$$

where the argument of the functions under the integrals is $\lambda x + (1 - \lambda) x_0$. For $0 < n < 2$ the integral in (6) is improper, the mean value theorem of differential calculus is used to justify

$$D_n \int_0^1 \lambda^{n/2-1} f \, d\lambda = \int_0^1 \lambda^{n/2-1} D_n f \, d\lambda. \tag{7}$$

If both y_1, y_2 solve $D_n y = f$ then the difference $y := y_1 - y_2$ obeys for $x \neq x_0$

$$2(x - x_0) \mid x - x_0 \mid^{-n/2} (\mid x - x_0 \mid^{n/2} y)' = D_n y = 0.$$

This proves the unicity $y = 0$, $y_1 = y_2$.

From now on, the potential $u = u(x)$ is assumed to be defined and smooth in some open interval.

Definition 1. *The two-point functions $Y_n = Y_n(x, x_0)$ $(n = 0, 1, 2, \ldots)$ are the unique smooth solutions in $(\mathrm{dom}\, u) \times (\mathrm{dom}\, u)$ of the differential-recursion scheme*

$$n D_{n-1} Y_n + L Y_{n-2} = 0 \qquad \text{for } n \geqq 2, \tag{8}$$

$$Y_0 := y_0, \qquad Y_1 := y_0'. \tag{9}$$

Here the differential operators D_{n-1}, L refer to the first argument x.

According to proposition 1, we may formally write

$$Y_n = -(n D_{n-1})^{-1} L Y_{n-2} \qquad \text{for } n \geqq 2$$

and the linear operator D_{n-1}^{-1} does not diminish the domain of definition and smoothness; therefore $\mathrm{dom}\, Y_n$ can be chosen independent of n. The recursion (8), (9) starts with constant functions Y_0, Y_1 and decomposes into subschemes for Y_{2m} $(m = 0, 1, 2, \ldots)$ and Y_{2m+1} $(m = 0, 1, 2, \ldots)$ respectively.

Let us now consider the general initial-value problem

$$Ly = 0, \; y(x_0) = y_0, \; y'(x_0) = y_0', \tag{10}$$

together with the special initial-value problems

$$L y_+ = 0, \; y_+(x_0) = y_0, \; y_+'(x_0) = 0, \tag{11}$$

$$L y_- = 0, \; y_-(x_0) = 0, \; y_-'(x_0) = y_0'. \tag{12}$$

For each $x_0 \in \mathrm{dom}\, u$ the problems (11), (12) admit unique smooth solutions $y_+ = y_+(x)$, $y_- = y_-(x)$ in some open subinterval $\mathrm{dom}\, y_+$, $\mathrm{dom}\, y_-$ respectively of $\mathrm{dom}\, u$. These compose to a solution of problem (10)

$$y := y_+ + y_- \quad \text{in} \quad \mathrm{dom}\, y := (\mathrm{dom}\, y_+) \cap (\mathrm{dom}\, y_-).$$

Definition 2. *The two-point functions $R_n = R_n(x, x_0)$ $(n = 0, 1, 2, \ldots)$ are the unique smooth solutions of the differential-recursion scheme*

(13) $$(n-2)\,D_{n+1}R_n + LR_{n-2} = 0 \qquad \text{for } n \geqq 3,$$

(14) $$R_0 := y_+, \qquad (x-x_0)\,R_1 := y_-,$$
$$(x-x_0)^2\,R_2 := y_+ - y_0.$$

Here the differential operators D_{n+1}, L refer to the first argument x.

Taylor's theorem applied to y_+, y_- shows that the start conditions (14) define smooth functions R_0, R_1, R_2 indeed. We may formally write

$$R_n = -((n-2)\,D_{n+1})^{-1}\,LR_{n-2} \qquad \text{for } n \geqq 3.$$

The recursion equation (13) decomposes into a separate equation for R_{2m} ($m = 0, 1, 2, \ldots$) and another for R_{2m+1} ($m = 0, 1, 2, \ldots$). For fixed $x_0 \in dom\,u$ we can take independent of $m = 0, 1, 2, \ldots$

$$dom\,R_{2m}(.,x_0) = dom\,y_+,\, dom\,R_{2m+1}(.,x_0) = dom\,y_-.$$

Theorem 1. *For each $m = 0, 1, 2, \ldots$ there holds*

(15) $$y_+ = \sum_{k=0}^{m-1} Y_{2k}\cdot(x-x_0)^{2k} + R_{2m}\cdot(x-x_0)^{2m},$$

(16) $$y_- = \sum_{k=0}^{m-1} Y_{2k+1}\cdot(x-x_0)^{2k+1} + R_{2m+1}\cdot(x-x_0)^{2m+1}.$$

As a consequence, for each $n = 0, 1, 2, \ldots$ there holds

(17) $$y = \sum_{k=0}^{n-1} Y_k\cdot(x-x_0)^k + R_n\cdot(x-x_0)^n.$$

Proof. We show that the two-point functions

$$Z_n := R_n - (x-x_0)^2\,R_{n+2} \qquad \text{for } n \geqq 2$$

fulfil the defining equations (8), (9) of the Y_n. Considering that

$$D_{n-1}Z_n = D_{n-1}R_n - (x-x_0)^2\,D_{n+3}R_{n+2},$$
$$LZ_{n-2} = LR_{n-2} - 2D_1R_n - (x-x_0)^2\,LR_n,$$
$$nD_{n-1}R_n - 2D_1R_n = (n-2)\,D_{n+1}R_n,$$

we obtain for $n \geqq 2$

$$nD_{n-1}Z_n + LZ_{n-2} =$$
$$= (n-2)\,D_{n+1}R_n + LR_{n-2} - (x-x_0)^2\,(nD_{n+3}R_{n+2} + LR_n) = 0.$$

The start condition $Z_0 = y_0$ directly follows from (14), while the calculation

$$D_0Z_1 = D_0R_1 - (x-x_0)^2\,D_4R_3 = D_0R_1 + (x-x_0)^2\,LR_1 =$$
$$= (x-x_0)\,L((x-x_0)\,R_1) = (x-x_0)\,Ly_- = 0$$

shows that

$$Z_1 = \text{const} = R_1(x_0, x_0) = y_0'.$$

Since the system (8), (9) has only one solution, there holds for $n = 0, 1, 2, \ldots, Z_n = Y_n$ or

$$R_n = Y_n + (x - x_0)^2 R_{n+2}.$$

Now a simple mathematical induction gives

$$R_0 = \sum_{k=0}^{m-1} Y_{2k} \cdot (x - x_0)^{2k} + R_{2m} \cdot (x - x_0)^{2m},$$

$$R_1 = \sum_{k=0}^{m-1} Y_{2k+1} \cdot (x - x_0)^{2k} + R_{2m+1} \cdot (x - x_0)^{2m},$$

which is equivalent to (15), (16).

We have just derived asymptotic expansions for $x \to x_0$

$$y_+ \sim \sum_{m=0}^{\infty} Y_{2m} \cdot (x - x_0)^{2m},$$

$$y_- \sim \sum_{m=0}^{\infty} Y_{2m+1} \cdot (x - x_0)^{2m+1},$$

$$y \sim \sum_{n=0}^{\infty} Y_n \cdot (x - x_0)^n.$$

These will convert into representations of functions by convergent series

(18) $$y_+ = \sum_{m=0}^{\infty} Y_{2m} \cdot (x - x_0)^{2m},$$

(19) $$y_- = \sum_{m=0}^{\infty} Y_{2m+1} \cdot (x - x_0)^{2m+1},$$

(20) $$y = \sum_{n=0}^{\infty} Y_n \cdot (x - x_0)^n$$

in two situations:

(i) If $u = u(x)$ is analytic then (18), (19), (20) represent analytic functions for sufficiently small $|x - x_0|$.

(ii) If some function Y_{2m} or Y_{2m+1} vanishes then all the following terms Y_{2k} or Y_{2k+1} respectively for $k = m + 1, m + 2, \ldots$ vanish too and the series (18) or (19) reduces to a finite sum.

A version of (i) is made precise by

Theorem 2. *Let the potential $u = u(x)$ be defined and analytic in some open interval. Then each $Y_n = Y_n(x, x_0)$ $(n = 0, 1, 2, \ldots)$ is defined and analytic in* *(dom u)* $\times$ *(dom u). Further, there exists a neighbourhood of the diagonal of (dom u)* $\times$ $\times$ *(dom u) where the series (20) converges and represents an analytic solution of the initial-value problem (10).*

Sketch of the proof. The linear operators D_n, D_n^{-1}, L act in the space of two-point functions which are defined and analytic in *(dom u)* $\times$ *(dom u)*. The lowest terms Y_0 and Y_1 are constant functions and therefore analytic, the analyticity of

$$Y_n = -(nD_{n-1})^{-1} L Y_{n-2} \qquad \text{for } n \geqq 2$$

follows by mathematical induction. The convergence of the series (20) for points x, x_0 which are sufficiently near to each other can be shown by means of the "method of majorants" in analogy to J. Hadamard's construction of the elementary solution to a second order linear partial differential operator with analytic coefficients [3]. We omit the details because only technical modifications are necessary to adopt the method to the present situation. Finally, it is verified that (20) solves (10):

$$Ly = \sum_{n=2}^{\infty} (nD_{n-1} Y_n + LY_{n-2}) (x - x_0)^{n-2} = 0;$$

the initial conditions are obvious.

EXAMPLES

1. If the potential is u = const = $\pm\omega^2 = 0$ then it is easy to find

$$Y_{2m} = \frac{u^m}{(2m)!} y_0, \qquad Y_{2m+1} = \frac{u^m}{(2m+1)!} y_0' \qquad \text{for } m = 0, 1, 2, \ldots$$

With this, the problem

$$y'' + \omega^2 y = 0, \omega \neq 0, y(0) = y_0, y'(0) = y_0'$$

is solved by

$$y = \sum_{n=0}^{\infty} Y_n \cdot x^n = y_0 \cos \omega x + y_0' \omega^{-1} \sin \omega x.$$

Analogously, the problem

$$y'' - \omega^2 y = 0, \omega \neq 0, y(0) = y_0, y'(0) = y_0'$$

is solved by

$$y = \sum_{n=0}^{\infty} Y_n \cdot x^n = y_0 \cosh \omega x + y_0' \omega^{-1} \sinh \omega x.$$

2. For the operator

$$L = \left(\frac{\mathrm{d}}{\mathrm{d}x} - \frac{n}{x}\right)\left(\frac{\mathrm{d}}{\mathrm{d}x} + \frac{n}{x}\right) = \frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{n(n+1)}{x^2}$$

mathematical induction shows

$$(2m+1)\binom{2m}{m} Y_{2m+1} = \binom{n}{m}\binom{n+m}{m} x^{-m} x_0^{-m} y_0',$$

Initial value problems are better solved directly, making use of the fundamental system x^{n+1}, x^{-n} of solutions of $Ly = 0$. If, particularly, n is a positive integer then $Y_{2m+1} = 0$ for $m \geqq n+1$. The example may be slightly generalized by a translation $x \mapsto x - x_1$, $x_0 \mapsto x_0 - x_1$.

We have been able to find all potentials $u = u(x)$ satisfying $Y_4(x, 0) \equiv 0$ or $Y_5(x, 0) \equiv 0$ respectively. For these the expansions (18), (19) shrink to

$$y_+ = y_0 + Y_2(x, 0)\, x^2 \qquad \text{or} \qquad y_- = y_0' x + Y_3(x, 0)\, x^3$$

respectively and produce explicit solutions in terms of elementary functions and Bessel functions. We omit this list of potentials and present under 3. and 4. two simple cases only. Clearly, the examples could be treated by verification or by other methods. They serve here to illustrate our theoretical results. Note that each of the conditions $Y_2(x, 0) \equiv 0$ or $Y_3(x, 0) \equiv 0$ implies vanishing potential $u(x) \equiv 0$, i.e. does not produce new examples.

3. The problem

$$\left(\frac{\mathrm{d}}{\mathrm{d}x} - v\right)\left(\frac{\mathrm{d}}{\mathrm{d}x} + v\right) y = 0, \qquad v := 2x(x^2 + a)^{-1},$$

$$y(0) = 1,\ y'(0) = 0,\ a = \text{const} \neq 0,$$

is solved by

$$u(x) = 2(3x^2 - a)(x^2 + a)^{-2},$$

$$Y_2(x, 0) = -(x^2 + a)^{-1}, \qquad Y_4(x, 0) = 0,$$

$$y = a(x^2 + a)^{-1}.$$

4. The problem

$$y'' - 6x(x^3 - 2a)(x^3 + a)^{-2}\, y = 0,$$

$$y(0) = 0, \qquad y'(0) = 1, \qquad a = \text{const} \neq 0,$$

is solved by

$$Y_3(x, 0) = -x(x^3 + a)^{-1}, \qquad Y_5(x, 0) = 0,$$

$$y = ax(x^3 + a)^{-1}.$$

5. Let us insert the one-soliton solution

$$u(x, t) = 2\omega^2 \cosh^{-2}(\omega x + 4\omega^3 t)$$

of the Korteweg-de Vries equation

$$\frac{\partial u}{\partial t} = 6u\frac{\partial u}{\partial x} + \frac{\partial^3 u}{\partial x^3}$$

into the linear initial-value problem

$$y'' + uy = 0,\ y(x_0) = 0,\ y'(x_0) = y_0'.$$

Solving $3D_2 Y_3 + LY_1 = 0$ for $Y_3 = Y_3(x, x_0)$ we obtain

$$6(x - x_0)\, Y_3 = y_0' \int_{x_0}^{x} u(z, t)\, dz =$$
$$= 2y_0'\omega[\tanh(\omega x + 4\omega^3 t) - \tanh(\omega x_0 + 4\omega^3 t)]$$

and with this and some smooth two-point function $R_5 = R_5(x, x_0)$ a representation

$$y = y_0'(x - x_0) + Y_3 \cdot (x - x_0)^3 + R_5 \cdot (x - x_0)^5.$$

6. J. L. Burchnall and T. W. Chaundy [2] established in 1929 that the differential-recursion scheme

$$\frac{d}{dx}\left(\frac{P_{n+1}}{P_{n-1}}\right) = (2n-1)\left(\frac{P_n}{P_{n-1}}\right)^2, \qquad P_1 := 1,\ P_2 := x + a_1$$

can be solved by polynomials $P_n = P_n(x)$ of degree $\binom{n}{2}$ with highest term $x^{\binom{n}{2}}$. This remarkable fact has been rediscovered at least twice [5, 1]. The n-th polynomial depends on $n - 1$ integration constants:

$$P_n = P_n(x + a_1, a_2, \ldots, a_{n-1}).$$

M. Adler and J. Moser [1] calculated in the normalization $a_1 = 0$

$$P_3 = x^3 + a_2, \qquad P_4 = x^6 + 5a_2x^3 + a_3x - 5a_2^2,$$

$$P_5 = x^{10} + 15a_2x^7 + 7a_3x^5 - 35a_2a_3x^2 + 175a_2^3x - \frac{7}{3}a_3^2 + a_4x^3 + a_4a_2.$$

J. E. Lagnese [5] established a theorem which can in our context be reformulated as follows: $Y_{2m+1} = 0$ identically in x, x_0, y_0' if and only if there exist an $n \leq m$ and a polynomial P_n such that

$$u(x) = 2\frac{d^2}{dx^2}\log P_n(x).$$

Then the initial-value problem

$$Ly = 0,\ y(x_0) = 0,\ y'(x_0) = y'_0$$

is solved by the finite sum

$$y = \sum_{k=0}^{m-1} Y_{2k+1} \cdot (x - x_0)^{2k+1}.$$

In the earlier paper [4] J. E. Lagnese treated (using other notations, of course) the example

$$P_3(x) = x^3 - 1, \qquad u(x) = 2\frac{d^2}{dx^2}\log P_3(x);$$

he explicitly calculated Y_3 and Y_5. We recognize our example 4 with $a = -1$.

For the trivial choice of the parameters our example 2 emerges from Lagnese's theorem [5]:

$$P_{n+1}(x) = x^{n(n+1)/2}, \qquad u(x) = -n(n+1)\,x^{-2}.$$

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