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Exact solution of the Schrödinger equation for a potential well with a barrier and other potentials

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Abstract. A method is described, with which exactly solvable, one-dimensional, stationary Schrödinger equations can be derived from solved differential equations. The procedure is illustrated by the example of a Schrödinger equation for a potential well with a barrier of the form

$$U(z) = \hat{v}\left(\hat{q}_2 \tanh^2 z + \hat{q}_1 \frac{\tanh z}{\cosh z} + \hat{q}_0\right).$$

The eigenvalues and eigenfunctions of this potential are calculated exactly. The results are explicit, analytical expressions in closed form for the whole eigenvalue spectrum as well as for all the eigenfunctions.

1. Introduction

For a long time exactly solvable Schrödinger equations have been the object of many investigations. An exact solution can usually be found only for special, simple potentials. In this paper a method is described, with which the Schrödinger equation can be solved exactly for relatively general potentials. The potentials may contain up to 11 arbitrary algebraic parameters.

Many exactly solvable potentials are polynomials or hyperbolic functions of the spatial coordinate. A potential well with finite walls, represented by a polynomial of second degree of $\tanh z$ (z is a dimensionless spatial coordinate), belongs to the hyperbolic case. This potential was discussed in detail by Morse and Feshbach [1]. For this well the eigenvalues and eigenfunctions are given in closed form. Compared with the harmonic oscillator this potential well has the virtue that it has a discrete, as well as a continuous, spectrum because of its finite depth. The great flexibility of this potential in relation to its simplicity was the reason for the careful investigation of these potentials, which are functions of $\tanh z$.

In section 2 a rational function of $\tanh z$ is permitted as potential. The Schrödinger equation with this potential is transformed by the same transformation with which the simple well was solved in [1]. The resulting differential equation is exactly solved by power series. The transformed Schrödinger equation has only regular singularities, if potentials with unfavourably lying poles are excluded. In this case the eigenvalue condition can be derived exactly.

Unfortunately it can only be solved for special cases of the general potential. In order to continue with the general calculations, the potential is restricted and the

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transformation is generalised. In the first step only symmetric potentials are considered. These are rational functions in $\tanh^2 z$. A special case of these potentials was discussed by Hudák and Trlifaj [7]. The Schrödinger equation is transformed by a transformation that takes advantage of the symmetry. The resulting differential equation has only regular singularities like that in the general case. The exact solutions of this differential equation are power series that are simpler than those of the general potential. The decisive change occurs in the eigenvalue condition. For symmetric potentials it is divided into two conditions. One of them produces the eigenvalues with even quantum number and the other the eigenvalues with odd quantum number. Unfortunately these eigenvalue conditions could not be solved in general, either. Therefore, in a second step, the general potential is further specialised.

It is not obvious how to restrict the general potential and how to guarantee simultaneously that the Schrödinger equation is exactly solvable. Therefore the method is slightly modified. The Schrödinger equation with a general potential is transformed generally. Explicit transformations and the appropriate potentials then follow from the requirement that the transformed differential equation is exactly solvable. Of course each of these potentials contains arbitrary algebraic parameters so that it represents a whole family of potentials. Nevertheless they are referred to as one potential.

Due to the restriction on these special potentials it is possible to solve the Schrödinger equation exactly. For all the potentials, which have been investigated until now, the eigenvalue condition can be solved for the eigenvalues explicitly and analytically. All eigenfunctions are given in closed form. Twenty four potentials are now known. In addition, all these potentials can be treated with the general method. The eigenvalues are, therefore, exact solutions of the general eigenvalue condition.

In section 2 the general method is described using as a potential a rational function of $\tanh z$. The calculations with the special potentials are, of course, more complicated than those with the general potential, because they result in explicit solutions. Therefore, it is suitable to solve the Schrödinger equation in two steps. The transformation, and thus the method of solution, is found and the appropriate potential is determined first (section 3). Afterwards the solution is determined explicitly. In section 4 the procedure is demonstrated for a potential well with a barrier.

2. Solution of the Schrödinger equation by series

2.1. General potential

2.1.1. Solution of the Schrödinger equation. In this section the general solution of the Schrödinger equation with a general potential is determined. The method of solution is a generalisation of the method used by Morse and Feschbach to solve the Schrödinger equation with a potential well with finite walls [1]. The Schrödinger equation is transformed into a differential equation with regular singularities, the exact solutions of which are power series.

A rational function of $\tanh z$ is chosen as a potential†:

$$U(z)=\frac{U_Z(z)}{U_N(z)} \qquad z=\frac{x}{d} \quad \text{dimensionless spatial coordinate}$$

$$\begin{aligned} U_Z(z)&=q_{Zn}\tanh^n z+q_{Zn-1}\tanh^{n-1} z+\ldots+q_{Z0} \\ U_N(z)&=q_{Nm}\tanh^m z+q_{Nm-1}\tanh^{m-1} z+\ldots+q_{N0}. \end{aligned} \tag{2.1}$$

† The subscript notation Z and N denotes Zähler (numerator), Nenner (denominator) respectively.

Up to now the zeros of $U_N(z)$ are arbitrary. Hence, (2.1) also contains potentials with poles. The potential well solved by Morse and Feshbach [1]

$$U_{\mathrm{MF}}(z) = q_{Z2}\tanh^2 z + q_{Z1}\tanh z + q_{Z0} \tag{2.2}$$

is a special case of (2.1). The dimensionless Schrödinger equation

$$\begin{aligned}
&\frac{d^2\varphi}{dz^2} + [\varepsilon - vU(z)]\varphi(z) = 0 \\
&v = \frac{2m\,d^2}{\hbar^2}U_0 \qquad \text{dimensionless potential depth} \\
&\varepsilon = \frac{2m\,d^2}{\hbar^2}E \qquad \text{dimensionless eigenvalue}
\end{aligned} \tag{2.3}$$

is transformed by

$$z = \tanh^{-1}(1-2u) \tag{2.4}$$

in a differential equation with rational coefficients. Its normal form is given by

$$u^2(1-u)^2\frac{d^2\varphi}{du^2} + \tfrac{1}{4}[1 + \varepsilon - vU(u)]\varphi(u) = 0. \tag{2.5}$$

The transformation (2.4) maps the real axis into the interval [0, 1]. In particular, $z = +\infty$ and $z = -\infty$ are transformed into $u = 0$ and $u = 1$, respectively. In (2.3) v is factored out, because the physical quantities (mass m and so on) are contained only in this parameter. $U(u)$ is the transformed potential

$$\begin{aligned}
&U(u) = U_Z(u)/U_N(u) \\
&U_Z(u) = Q_{Zn}u^n + Q_{Zn-1}u^{n-1} + \ldots + Q_{Z0} \\
&U_N(u) = Q_{Nm}u^m + Q_{Nm-1}u^{m-1} + \ldots + Q_{N0}.
\end{aligned} \tag{2.6}$$

Its coefficients are defined by

$$\begin{aligned}
&Q_{Ak} = (-2)^k \sum_{j=0}^{p} \binom{j}{k} q_{Aj} \qquad A \in \{Z, N\} \\
&p = \begin{cases} n & \text{for } A = Z \\ m & \text{for } A = N. \end{cases}
\end{aligned} \tag{2.7}$$

Differential equations with rational coefficients may often be solved by power series. The power series expansion is prepared by the transformation [4]

$$\varphi(u) = u^{1/2+\lambda_1}(1-u)^{1/2+\lambda_2}y(u) \tag{2.8}$$

whereby

$$\begin{aligned}
&\lambda_1 = \tfrac{1}{2}[vU(z = +\infty) - \varepsilon]^{1/2} \\
&\lambda_2 = \tfrac{1}{2}[vU(z = -\infty) - \varepsilon]^{1/2}.
\end{aligned} \tag{2.9}$$

The differential equation (2.5) is transformed by (2.8) into

$$u(1-u)U_N(u)\frac{d^2y}{du^2}+(b_1u+b_0)U_N(u)\frac{dy}{du}$$
$$+\{-\tfrac{1}{4}b_1(b_1+2)U_N(u)+\tfrac{1}{4}v[U(u=0)U_{N0}(u)$$
$$+U(u=1)U_{N1}(u)-U_{Z01}(u)]\}y(u)=0 \tag{2.10}$$

whereby

$$b_0=2\lambda_1+1$$
$$b_1=-2(\lambda_1+\lambda_2+1) \tag{2.11}$$

and with the potential terms

$$U_{A0}(u)=\frac{U_A(u)-U_A(u=0)}{u}$$
$$U_{A1}(u)=\frac{U_A(u)-U_A(u=1)}{1-u} \qquad A\in\{Z,N\} \tag{2.12}$$
$$U_{A01}(u)=\frac{U_{A0}(u)-U_{A0}(u=1)}{1-u}.$$

In (2.12) all divisions can be worked out without there being remainder terms. Therefore, all expressions are polynomials. The solution of (2.10) is connected with the solution of the Schrödinger equation (2.3) by

$$\varphi(z)=u^{\lambda_1}(1-u)^{\lambda_2}y(u) \qquad u=\tfrac{1}{2}(1-\tanh z). \tag{2.13}$$

The factors in front of $y(u)$ represent the asymptotic behaviour of the solution. It is remarkable that an interchange of the transformations (2.4) and (2.8) complicates the calculations considerably.

The differential equation (2.10) has singularities at 0, 1 and at the zeros of the denominator of the transformed potential. In general, series expansions can be worked out without any difficulties only about regular singular points [4]. In section 2.1.2 the boundary conditions are used to determine the eigenvalue condition. Therefore an expansion about 0 or 1 (corresponding to $z=\pm\infty$) is suitable. The points 0 and 1 are regular, if the potential is bounded at infinity

$$U(z=\pm\infty)<\infty. \tag{2.14}$$

Condition (2.14) is assumed in the following.

The solution of (2.10) is expanded about 0:

$$y(u)=c_{p1}P_1(u)+c_{p2}u^{-2\lambda_1}P_2(u) \qquad u\in[0,r[$$
$$r=\min\{1,|u_k|\,|\,U_N(u_k)=0\} \tag{2.15}$$

where P_1 and P_2 are power series. Their radius of convergence is the minimal distance to the next singularity. The series are represented by

$$P_1(u)=\sum_{j=0}^{\infty}R_ju^j \tag{2.16}$$

$$P_2(u)=\sum_{j=0}^{\infty}\hat{R}_ju^j. \tag{2.17}$$

The coefficients of the series are defined by the recurrence relation

$$(j+1)(jA_1+B_0)R_{j+1}+[j(j-1)A_2+jB_1+C_0]R_j$$
$$+\ldots+[(j-m)(j-m-1)A_{m+2}+(j-m)B_{m+1}+C_m]R_{j-m}$$
$$+C_{m+1}R_{j-m-1}+\ldots+C_pR_{j-p}=0 \qquad (2.18)$$

$$R_j=R_j(\mu_0,\mu_1) \qquad R_{-j}=0 \text{ for } j>0$$

$$R_0=1 \qquad p=\max\{m, n-2\}$$

whereby

$$A_k=Q_{Nk-1}-Q_{Nk-2} \qquad 1\leqslant k\leqslant m+2 \qquad Q_{Nm+1}=Q_{N-1}=0 \qquad (2.19)$$

$$B_k=(1-\mu_0)Q_{Nk}+(\mu_1+\mu_0-2)Q_{Nk-1}$$
$$0\leqslant k\leqslant m+1 \qquad Q_{Nm+1}=Q_{N-1}=0 \qquad (2.20)$$

$$C_k=[\tfrac{1}{2}(1-\mu_0)(\mu_1-1)-\tfrac{1}{2}b_0(b_0+b_1)-\tfrac{1}{4}b_1(b_1+2)]Q_{Nk}$$
$$+\tfrac{1}{4}v\{-U(u=1)(Q_{Nm}+\ldots+Q_{Nk+2})$$
$$+[U(u=0)-U(u=1)]Q_{Nk+1}+(Q_{Zn}+\ldots+Q_{Zk+2})\} \qquad (2.21)$$

$$0\leqslant k\leqslant p \qquad Q_{Nk}=0 \text{ for } k>m \qquad Q_{Zk}=0 \text{ for } k>n.$$

The parameters μ_j determine which series is defined by (2.18)

$$R_j=R_j(\mu_0,\mu_1) \qquad \mu_0=1-b_0 \qquad \mu_1=1+b_0+b_1 \qquad (2.22)$$

$$\hat{R}_j=R_j(-\mu_0,\mu_1) \qquad \mu_0=1-b_0 \qquad \mu_1=1+b_0+b_1. \qquad (2.23)$$

The general solution of the Schrödinger equation with the potential (2.1) and the restriction (2.14) is given by

$$\varphi(z)=u^{\lambda_1}(1-u)^{\lambda_2}[c_{p1}P_1(u)+c_{p2}u^{-2\lambda_1}P_2(u)]$$
$$u\in[0,r[\qquad u=\tfrac{1}{2}(1-\tanh z). \qquad (2.24)$$

The equations (2.16) to (2.23) show how the parameters of the solution (2.24) depend on the parameters of the potential (2.1).

2.1.2. Eigenvalue condition. In this section the eigenvalue condition is derived exactly from the general solution of the Schrödinger equation (2.24). The potential has to be restricted at first to guarantee that all singularities of the differential equation (2.10) in the unit circle are regular. Then the solution (2.24) is continued to apply the boundary conditions. The eigenvalue condition is a consequence of the requirement that the solution has to vanish at infinity.

The general solution (2.24) was expanded about $u=0$ ($z=+\infty$). Hence the boundary condition at $z=+\infty$ can be applied directly to (2.24). In the asymptotic representation

$$\varphi(z)\to c_{p1}u^{\lambda_1}+c_{p2}u^{-\lambda_1} \qquad u\to 0 \qquad (2.25)$$

the second term diverges so that

$$c_{p2}=0. \qquad (2.26)$$

The boundary condition at $u=0$ cancels one of the two linearly independent solutions. The other boundary condition occurs at $u=1$ ($z=-\infty$). From the equations (2.24) and (2.15) it follows that this point does not lie in the circle of convergence of the series in the solution (2.24). Therefore, a representation of the series P_1 that is defined at $u=1$ has to be found. This is possible by the help of the analytic continuation of the series P_1 [6].

The differential equation must not have any irregular singularity in the unit circle in order to continue P_1 to $u=1$. This is the case, if the denominator of the transformed potential has only zeros at most of second order in the unit circle. In future this is assumed

$$\begin{aligned}&(\xi\in\mathbb{E}\wedge U_N(\xi)=0)\Rightarrow U_N(u)=(u-\xi)^k\bar{U}_N(u)\\&k\in\{1,2\}\wedge\bar{U}_N(\xi)\neq 0.\end{aligned}\tag{2.27}$$

It has to be pointed out that a potential (2.1) that is restricted by (2.27) and (2.14) may still have poles. Under these assumptions the series P_1 can be continued to $u=1$.

Condition (2.27) is a commensurate, but not a necessary, condition. If the singularities lie at convenient positions, P_1 can be continued under essentially weaker assumptions. In some cases even irregular singularities may lie in the unit circle. These cases cannot be discussed in general so that they are excluded by (2.27).

To simplify the future calculations, it is assumed that $U_N(u)$ has no singularity in the unit circle except at $u=0$. Then the analytic continuation of P_1 is given by

$$P_1(u)=\alpha P_3(u)+\beta(1-u)^{-2\lambda_2}P_4(u)\qquad u\in\,]0,1]\tag{2.28}$$

whereby α and β are unknown coefficients. P_3 and P_4 are power series expanded about $u=1$

$$P_3(u)=\sum_{j=0}^{\infty}\tilde{R}_j(1-u)^j\qquad \tilde{R}_0=1\tag{2.29}$$

$$P_4(u)=\sum_{j=0}^{\infty}\dot{R}_j(1-u)^j\qquad \dot{R}_0=1.\tag{2.30}$$

Considering (2.26) the solution of the Schrödinger equation is given by

$$\varphi(z)=c_{p1}u^{\lambda_1}(1-u)^{\lambda_2}[\alpha P_3(u)+\beta(1-u)^{-2\lambda_2}P_4(u)]\qquad u\in\,]0,1].\tag{2.31}$$

The asymptotic form of (2.31) is

$$\varphi(z)\to c_{p1}[\alpha(1-u)^{\lambda_2}+\beta(1-u)^{-\lambda_2}]\qquad u\to 1.\tag{2.32}$$

The second term diverges and the eigenvalue condition is given by

$$\beta(\varepsilon)=0.\tag{2.33}$$

To determine the unknown coefficient β, a result in a paper of Schäfke and Schmidt [2] is used. They prove that β can be expressed by the coefficients of the series P_1

$$\beta(\varepsilon)=\Gamma(-\mu_1)\lim_{j\to\infty}\frac{\Gamma(j+1)}{\Gamma(j-\mu_1)}R_j(\mu_0,\mu_1).\tag{2.34}$$

The eigenvalue condition of the potential (2.1) with the restriction (2.14) and under the assumption that $U_N(u)$ has no zero in the unit circle is given by

$$\lim_{j\to\infty}\frac{\Gamma(j+1)}{\Gamma(j-\mu_1)}R_j(\mu_0,\mu_1)=0.\tag{2.35}$$

For the sake of completeness the coefficient α is also given,

$$\alpha = \Gamma(\mu_1) \lim_{j\to\infty} \frac{\Gamma(j+1)}{\Gamma(j+\mu_1)} \bar{R}_j \tag{2.36}$$

where

$$\bar{R}_j = R_j(\mu_0, -\mu_1) \qquad \mu_0 = 1 - b_0 \qquad \mu_1 = 1 + b_0 + b_1. \tag{2.37}$$

A similar eigenvalue condition can be derived, if $U_N(u)$ satisfies only condition (2.27). Then an equation similar to (2.28) has to be used repeatedly. Starting at $u = 0$, the series is continued until $u = 1$ lies in the circle of convergence. Obviously the calculations proceed as described above. The coefficients of (2.32), however, are given by more complicated expressions. Thus, it is possible to derive a similar eigenvalue condition as (2.35) for the potential (2.1) under the assumptions (2.14) and (2.27).

2.2. *Symmetric potential*

2.2.1. Solution of the Schrödinger equation. The eigenvalue condition (2.35) cannot be solved in general. It is known that further results can be derived if the potential possesses special properties. Therefore only symmetric potentials are discussed in this section. To use the properties of these specialised potentials, the transformation (2.4) is generalised. The new transformation makes use of the symmetry. The method of solution is essentially the same as in section 2.1.1. The main difference is that the new transformation divides the interval into two parts. The most important result is that the recurrence relation, which defines the solution of the Schrödinger equation, contains only half as many terms as in the general case, if the polynomials of the potential are of the same degree. This is an essential simplification.

The symmetric potential

$$\begin{aligned} U_{\mathrm{S}}(z) &= \frac{U_{\mathrm{S}\,Z}(z)}{U_{\mathrm{S}\,N}(z)} \\ U_{\mathrm{S}\,Z}(z) &= q_{\mathrm{S}\,Z\,2n} \tanh^{2n} z + q_{\mathrm{S}\,Z\,2n-2} \tanh^{2n-2} z + \ldots + q_{\mathrm{S}\,Z\,0} \\ U_{\mathrm{S}\,N}(z) &= q_{\mathrm{S}\,N\,2m} \tanh^{2m} z + q_{\mathrm{S}\,N\,2m-2} \tanh^{2m-2} z + \ldots + q_{\mathrm{S}\,N\,0} \end{aligned} \tag{2.38}$$

contains only even powers of tanh z. A transformation taking this into account should depend on the square root of a linear function of u. Hence, the transformation

$$z = \tanh^{-1} \delta(1-u)^{1/2} \qquad \delta = \begin{cases} -1 & \text{for } z \leqslant 0 \\ 1 & \text{for } z \geqslant 0 \end{cases} \tag{2.39}$$

is used. This transformation maps the positive semiaxis as well as the negative semiaxis into the interval [0, 1]. In particular $z = \pm\infty$ is mapped into u=0. The ambiguity of δ at the origin is necessary to close both intervals. The transformation introduces a division of the interval so that two transformed differential equations correspond to the Schrödinger equation. The Schrödinger equation is transformed by (2.39) into

$$u^2(1-u)^2 \frac{\mathrm{d}^2\varphi}{\mathrm{d}u^2} + \tfrac{1}{4}\{\tfrac{3}{4}u^2 + (1-u)[1 + \varepsilon - vU_{\mathrm{S}}(u)]\}\varphi(u) = 0 \tag{2.40}$$

with the transformed potential

$$\begin{aligned} U_{\mathrm{S}}(u) &= U_{\mathrm{S}\,Z}(u)/U_{\mathrm{S}\,N}(u) \\ U_{\mathrm{S}\,Z}(u) &= Q_{\mathrm{S}\,Z\,n} u^n + Q_{\mathrm{S}\,Z\,n-1} u^{n-1} + \ldots + Q_{\mathrm{S}\,Z\,0} \\ U_{\mathrm{S}\,N}(u) &= Q_{\mathrm{S}\,N\,m} u^m + Q_{\mathrm{S}\,N\,m-1} u^{m-1} + \ldots + Q_{\mathrm{S}\,N\,0}. \end{aligned} \tag{2.41}$$

Its coefficients are defined by

$$Q_{\mathrm{S}Ak}=(-1)^k\sum_{j=k}^{p}\binom{j}{k}q_{Aj}\qquad A\in\{Z,N\}$$
$$p=\begin{cases}n & \text{for } A=Z\\ m & \text{for } A=N.\end{cases}\tag{2.42}$$

The degree of the polynomials $U_{\mathrm{S}Z}(u)$ and $U_{\mathrm{S}N}(u)$ is half as large as in (2.6). The parameter δ does not occur in the transformed Schrödinger equation (2.40). Therefore (2.40) is valid in both partial intervals and it is sufficient to solve (2.40).

Analogous to (2.8), (2.40) is transformed by

$$\varphi(u)=u^{1/2+\lambda_{\mathrm{S}1}}(1-u)^{1/4}y(u)\tag{2.43}$$

$$\lambda_{\mathrm{S}1}=\tfrac{1}{2}[vU_{\mathrm{S}}(z=\pm\infty)-\varepsilon]^{1/2}\tag{2.44}$$

into the differential equation

$$u(1-u)U_{\mathrm{S}N}(u)\frac{\mathrm{d}^2y}{\mathrm{d}u^2}+(b_{\mathrm{S}1}u+b_{\mathrm{S}0})U_{\mathrm{S}N}(u)\frac{\mathrm{d}y}{\mathrm{d}u}$$
$$+\{-\tfrac{1}{4}b_{\mathrm{S}0}(b_{\mathrm{S}0}-1)U_{\mathrm{S}N}(u)+\tfrac{1}{4}v[U_{\mathrm{S}}(u=0)U_{\mathrm{S}N0}(u)-U_{\mathrm{S}Z0}(u)]\}y(u)=0\tag{2.45}$$

whereby

$$b_{\mathrm{S}0}=2\lambda_{\mathrm{S}1}+1\qquad b_{\mathrm{S}1}=-(2\lambda_{\mathrm{S}1}+\tfrac{3}{2})=-(b_{\mathrm{S}0}+\tfrac{1}{2})\tag{2.46}$$

$$U_{\mathrm{S}A0}(u)=\frac{U_{\mathrm{S}A}(u)-U_{\mathrm{S}A}(u=0)}{u}\qquad A\in\{Z,N\}.\tag{2.47}$$

The expressions (2.47) are polynomials. The solutions y and φ are connected by

$$\varphi(z)=u^{\lambda_{\mathrm{S}1}}y(u)\qquad u=1-\tanh^2 z.\tag{2.48}$$

Due to the symmetry of the potential, the asymptotic behaviour of the solution of the Schrödinger equation is contained in the power of u. Under the transformation (2.39) the point $u=1$ is not a marginal point. Hence, the power of $1-u$ is missing in (2.48) compared with (2.13).

The differential equation (2.45) can be solved by a power series expansion, if 0 and 1 are regular singularities. This is the case, if $U_{\mathrm{S}}(z)$ is bounded at infinity and has a pole at most of second order at $z=0$:

$$U_{\mathrm{S}}(z=\pm\infty)<\infty$$
$$U_{\mathrm{S}N}(z)=\tanh^{2k}z\,\bar{U}_{\mathrm{S}N}(z)\qquad\text{with}\qquad \bar{U}_{\mathrm{S}N}(0)\neq 0\wedge 0\leqslant k\leqslant 1.\tag{2.49}$$

With symmetric potentials, there is an additional condition on the potential at $z=0$. The point $z=0$ is the link between both partial intervals. If the potential has a pole satisfying (2.49), a further transformation has to be worked out before expanding the solution. By the help of suitable substitutions the transformed differential equation can also be put into the form (2.45). Therefore, it can be assumed without loss of generality that $U_{\mathrm{S}N}(u)$ has no zero at $u=1$. The solution is expanded about $u=0$:

$$y(u)=c_{p\mathrm{S}1}P_{\mathrm{S}1}(u)+c_{p\mathrm{S}2}u^{-2\lambda_{\mathrm{S}1}}P_{\mathrm{S}2}(u)\qquad u\in[0,r[$$
$$r=\min\{1,|u_k|\,|\,U_{\mathrm{S}N}(u_k)=0\}.\tag{2.50}$$

Here P_{S1} and P_{S2} are power series,

$$P_{S1}(u)=\sum_{j=0}^{\infty} R_{Sj}u^j \tag{2.51}$$

$$P_{S2}(u)=\sum_{j=0}^{\infty} \widehat{R_{Sj}}u^j. \tag{2.52}$$

Their coefficients are defined by the recurrence relation

$$\begin{aligned}(j+1)(jA_{S1}+B_{S0})R_{Sj+1}&+[j(j-1)A_{S2}+jB_{S1}+C_{S0}]R_{Sj}\\ &+\ldots+[(j-m)(j-m-1)A_{Sm+2}+(j-m)B_{Sm+1}+C_{Sm}]R_{Sj-m}\\ &+C_{Sm+1}R_{Sj-m-1}+\ldots+C_{Sp}R_{Sj-p}=0 \qquad R_{Sj}=R_{Sj}(\mu_{S0},\mu_{S1})\end{aligned} \tag{2.53}$$

$R_{S-j}=0$ for $j>0$ $\qquad R_{S0}=1 \qquad p=\max\{m, n-1\}$

whereby

$$\begin{aligned}&A_{Sk}=Q_{SNk-1}-Q_{SNk-2} \qquad 1\leqslant k\leqslant m+2\\ &Q_{SNm+1}=Q_{SN-1}=0\end{aligned} \tag{2.54}$$

$$\begin{aligned}&B_{Sk}=(1-\mu_{S0})Q_{SNk}+(\mu_{S0}+\mu_{S1}-2)Q_{SNk-1}\\ &0\leqslant k\leqslant m+1 \qquad Q_{SNm+1}=Q_{SN-1}=0\end{aligned} \tag{2.55}$$

$$\begin{aligned}C_{Sk}=[\tfrac{1}{2}(1-\mu_{S0})(\mu_{S1}-1)-\tfrac{1}{4}b_{S0}(b_{S0}-2)]Q_{SNk}&\\ +\tfrac{1}{4}[U_S(u=0)Q_{SNk+1}-Q_{SZk+1}] \qquad 0\leqslant k\leqslant p&\end{aligned} \tag{2.56}$$

$Q_{SNk}=0$ for $k>m$ $\qquad Q_{SZk}=0$ for $k>n$.

The series are defined by

$$R_{Sj}=R_{Sj}(\mu_{S0},\mu_{S1}) \qquad \mu_{S0}=1-b_{S0} \qquad \mu_{S1}=\tfrac{1}{2} \tag{2.57}$$

$$\widehat{R_{Sj}}=R_{Sj}(-\mu_{S0},\mu_{S1}) \qquad \mu_{S0}=1-b_{S0} \qquad \mu_{S1}=\tfrac{1}{2}. \tag{2.58}$$

Obviously (2.53) contains only half as many terms compared with (2.18).

The general exact solution of the Schrödinger equation with the potential (2.38) and the restriction (2.49) is given by

$$\begin{aligned}&\varphi(z)=u^{\lambda_{S1}}[c_{pS1}P_{S1}(u)+c_{pS2}u^{-2\lambda_{S1}}P_{S2}(u)]\\ &u=1-\tanh^2 z \qquad u\in[0, r[.\end{aligned} \tag{2.59}$$

2.2.2. Eigenvalue condition. In this section the eigenvalue condition is exactly derived from the general solution (2.59) of the Schrödinger equation with a symmetric potential. As in the general case, the potential (2.38) has to be restricted so that the differential equation (2.45) has only regular singularities in the unit circle. Due to the symmetry of the potential, both boundary conditions are satisfied at the same time. The eigenvalue condition follows from fitting together the two partial solutions at $z=0$. This results in two eigenvalue conditions. One of them produces the eigenvalues with even quantum numbers and the other those with odd quantum numbers.

The general solution (2.59) is expanded about $u = 0$. On account of the transformation (2.39), this point corresponds to $z = \pm\infty$. Therefore, both boundary conditions can be considered at the same time. In the asymptotic representation

$$\varphi(z) \to c_{pS1} u^{\lambda_{S1}} + c_{pS2} u^{-\lambda_{S1}} \qquad u \to 0 \tag{2.60}$$

the second term diverges, and therefore

$$c_{pS2} = 0. \tag{2.61}$$

The transformation (2.39) introduces a division of the interval. The solution of the Schrödinger equation, therefore, consists of two parts

$$\begin{aligned} \varphi_+(z) &= c_{pS1+} u^{\lambda_{S1}} P_{S1}(u) \qquad && z \geqslant 0 \\ \varphi_-(z) &= c_{pS1-} u^{\lambda_{S1}} P_{S1}(u) \qquad && z \leqslant 0 \\ u &= 1 - \tanh^2 z \qquad && u \in [0, r[. \end{aligned} \tag{2.62}$$

The wavefunction has to be continuously differentiable at $z = 0$ $(u = 1)$. To fit together both partial solutions, they first have to be continued to $u = 1$. This is possible, if $U_{SN}(u)$ has only zeros at most of second order in the unit circle ((2.27)). As in the general case it is assumed for the sake of simplicity that $U_{SN}(u)$ has no zeros in the unit circle. Then $P_{S1}(u)$ can be directly continued to $u = 1$:

$$P_{S1}(u) = \alpha_S P_{S3}(u) + \beta_S (1-u)^{1/2} P_{S4}(u) \qquad u \in]0, 1] \tag{2.63}$$

whereby

$$P_{S3}(u) = \sum_{j=0}^{\infty} \widetilde{R_{Sj}} (1-u)^j \qquad \widetilde{R_{S0}} = 1 \tag{2.64}$$

$$P_{S4}(u) = \sum_{j=0}^{\infty} \dot{R}_{Sj} (1-u)^j \qquad \dot{R}_{S0} = 1. \tag{2.65}$$

The series P_{S1} is continued to $u = 1$. Then the solution of the Schrödinger equation, considering (2.61), is given by

$$\varphi(z) = c_{pS1} u^{\lambda_{S1}} [\alpha_S P_{S3}(u) + \beta_S (1-u)^{1/2} P_{S4}(u)] \qquad u \in]0, 1]. \tag{2.66}$$

The asymptotic representations of both partial solutions are a consequence of (2.66)

$$\begin{aligned} \varphi_+(z) &\to c_{pS1+} \alpha_S \\ \varphi_-(z) &\to c_{pS1-} \alpha_S \end{aligned} \qquad u \to 1. \tag{2.67}$$

The derivative of (2.66) is

$$\begin{aligned} \frac{d\varphi}{dz} = -2 c_{pS1} \delta u^{\lambda_{S1}} \Bigg[& \lambda_{S1} (1-u)^{1/2} [\alpha_S P_{S3}(u) + \beta_S (1-u)^{1/2} P_{S4}(u)] \\ & + u \left(\alpha_S (1-u)^{1/2} \frac{d}{du} P_{S3} - \tfrac{1}{2} \beta_S P_{S4}(u) + \beta_S (1-u) \frac{d}{du} P_{S4} \right) \Bigg]. \end{aligned} \tag{2.68}$$

Equation (2.68) depends on δ. Only at this place is the division of the interval explicitly expressed. The limits of the derivatives are given by

$$\begin{aligned} \varphi_+(z) &\to c_{pS1+} \beta_S \\ \varphi_-(z) &\to -c_{pS1-} \beta_S \end{aligned} \qquad u \to 1. \tag{2.69}$$

Thus the conditions of continuity are given by

$$c_{pS1+}\alpha_S = c_{pS1-}\alpha_S \tag{2.70}$$

$$c_{pS1+}\beta_S = -c_{pS1-}\beta_S. \tag{2.71}$$

To solve this system, the cases $\alpha_S = 0$ and $\alpha_S \neq 0$ have to be distinguished. α_S and β_S must not vanish simultaneously, since this would be a violation of the linear independence of the series P_{S1} and P_{S2}, because of (2.66) and (2.59). Hence, the eigenvalue condition follows:

$$\alpha_S(\varepsilon) = 0 \Rightarrow c_{pS1+} = -c_{pS1-} \qquad \text{(odd)} \tag{2.72}$$

$$\alpha_S \neq 0 \Rightarrow c_{pS1+} = c_{pS1-} \Rightarrow \beta_S(\varepsilon) = 0 \qquad \text{(even)}. \tag{2.73}$$

There are two eigenvalue conditions with symmetric potentials. One of them produces the even eigenvalues and the other the odd ones. By (2.72) and (2.73), the symmetry of the eigenfunctions is also obvious. As in the general case, α_S and β_S can be expressed by the coefficients of the series P_{S1}:

$$\alpha_S = \sqrt{\pi} \lim_{j\to\infty} \frac{\Gamma(j+1)}{\Gamma(j+\frac{1}{2})} R_{Sj}(\mu_{S0}, -\mu_{S1}) \tag{2.74}$$

$$\beta_S = -2\sqrt{\pi} \lim_{j\to\infty} \frac{\Gamma(j+1)}{\Gamma(j-\frac{1}{2})} R_{Sj}(\mu_{S0}, \mu_{S1}). \tag{2.75}$$

3. Solution of the Schrödinger equation by transformation

3.1. General transformation of the Schrödinger equation

In this section Schrödinger equations with the potential (2.1) are investigated, which are exactly solvable. To achieve this, the potential has to be restricted in a suitable way. Since it is not obvious how the potential is connected with the requirement of exact solvability, a general function of the spatial coordinate is used as a potential. Then the Schrödinger equation with this potential is transformed by a similar general transformation. The differential equation so derived is to be exactly solvable. From this requirement special transformations and the appropriate potentials can be calculated explicitly.

The dimensionless Schrödinger equation

$$\frac{d^2\varphi}{dz^2} + [\varepsilon - U(z)]\varphi(z) = 0 \tag{3.1}$$

is transformed by

$$z = g(x). \tag{3.2}$$

The normal form of the resulting differential equation is as follows:

$$\frac{d^2y}{dx^2} + \left[\frac{1}{2}\frac{g'''}{g'} - \frac{3}{4}\left(\frac{g''}{g'}\right)^2 + [\varepsilon - U(x)]g'^2\right] y(x) = 0. \tag{3.3}$$

This differential equation is to be solvable exactly, that is the invariant of (3.3)

$$I(x) = \frac{1}{2}\frac{g'''}{g'} - \frac{3}{4}\left(\frac{g''}{g'}\right)^2 + [\varepsilon - U(x)]g'^2 \tag{3.4}$$

has to be identical with that of a solved differential equation. In principle each differential equation that contains at least one algebraic parameter (eigenvalue), is permitted for this purpose. To simplify the further calculations, only such differential equations are considered that most probably produce usable Schrödinger equations. Furthermore, the solved differential equation should contain as many algebraic parameters as possible. Therefore, the hypergeometric differential equation (potential (2.2)), Whittaker's differential equation [4] and the differential equation of the harmonic oscillator are considered. The formal similarities of these differential equations permit a common treatment.

Requiring that (3.4) is identical with the invariant of these differential equations we have

$$I(x) = P_2(x)/Q_3^2(x) \tag{3.5}$$

where P_2 and Q_3 are polynomials of x of second and third degree, respectively, with arbitrary coefficients. The invariant (3.5) contains that of the hypergeometric differential equation. A certain similarity of this method with Sommerfeld's polynomial method [3] follows from this property. The coefficients of Q_3 are connected to the solvable differential equation by

$$Q_3(x) = q_3x^3 + q_2x^2 + q_1x + q_0 \tag{3.6}$$

with the following special cases:

(i) hypergeometric differential equation transformed with $1(ax+b)$

$$q_3 \neq 0$$

(ii) hypergeometric differential equation

$$q_3 = 0 \qquad q_2 \neq 0$$

(iii) Whittaker's differential equation

$$q_3 = q_2 = 0 \qquad q_1 \neq 0$$

(iv) harmonic oscillator

$$q_3 = q_2 = q_1 = 0 \qquad q_0 \neq 0.$$

The potential can be determined from (3.5). It is given by

$$\varepsilon - U(x) = \frac{P_2}{Q_3^2}\frac{1}{g'^2} - \left[\frac{1}{2}\frac{g'''}{g'} - \frac{3}{4}\left(\frac{g''}{g'}\right)^2\right]\frac{1}{g'^2}. \tag{3.7}$$

In (3.7) $g(x)$ and $U(x)$ are arbitrary functions. In particular, it is possible to calculate U for each g so that (3.5) is satisfied and therefore the appropriate differential equation is exactly solvable. The other case, in which the potential U is given and a transformation g is derived from (3.7), would be more interesting. Unfortunately, (3.7) is an unsolvable differential equation for $g(x)$.

The left-hand side of equation (3.7) is a difference of a constant (eigenvalue) and a function (potential) that does not depend on this constant. Therefore, the transformation g has to be chosen in such a way that the right-hand side of (3.7) is of the same form. Due to the complicated dependence of (3.7) on g, it is not easy to find suitable transformations. If, nevertheless, a transformation is found so that one of its parameters produces the eigenvalue, a new problem occurs. Equation (3.7) represents the transformed potential $U(x)$. To determine $U(z)$, x has to be eliminated by (3.2). Hence $U(z)$ becomes dependent on the eigenvalue, because g should produce the eigenvalue.

There is an alternative if the calculations are not worked out as general as possible. Then the requirement is that P_2 is to produce the eigenvalue. Since the parameters of P_2 occur nowhere else in the expression (3.7), it is guaranteed that the remainder does not depend on the eigenvalue. Then the backward transformation does not depend on the eigenvalue either. This requirement is satisfied, if the relation

$$\frac{1}{Q_3^2 g'^2} = \frac{1}{R_2} \tag{3.8}$$

holds. R_2 is a polynomial of second degree in x. In this case after working out the polynomial division P_2/R_2 the first term in (3.7) produces a constant, which contains a parameter of P_2. The differential equation (3.8) can be solved for g,

$$g(x) = \int \frac{[R_2(x)]^{1/2}}{Q_3(x)} \, \mathrm{d}x. \tag{3.9}$$

Therefore the transformation (3.9) yields with a potential given by (3.7) exactly solvable Schrödinger equations. R_2 and Q_3 are polynomials of second and third degree, respectively, with arbitrary algebraic coefficients.

The transformations (3.9) are of a relatively special form. To derive more general transformations or transformations of another form, other differential equations than those considered in (3.5) and (3.6) can be investigated. The calculations, however, become considerably more complicated.

The potential (3.7) determines the Schrödinger equation and the transformation (3.9) determines the appropriate method of solution. To obtain the solution explicitly, the polynomials have to be substituted in (3.9) and the integration has to be performed. It is convenient to treat separate cases to perform the integration.

3.2. *Special transformations*

On account of the many algebraic parameters, the investigation of the general transformation (3.9) and of the appropriate potential (3.7) is very complicated. Therefore, explicit polynomials are substituted for R_2 and Q_3 in (3.9) so that the integration can be performed. Since the transformations are expected to give new insight into the method described in section 2, only those transformations are discussed, which are inverse hyperbolic functions of x, after having worked out the integration.

These transformations can be put in the form

$$g(x) = \tanh^{-1} \frac{f(x) - 1}{f(x) + 1}. \tag{3.10}$$

The special form of the argument of $\tanh^{-1}$ does not result in a loss of generality, but is convenient for the calculation of the potential (3.7). For example, $f(x)$ stands for the following functions:

$$f(x) = (ax + b)^c \tag{3.11}$$

$$f(x) = d[2\sqrt{a}(ax^2 + bx + c)^{1/2} + 2ax + b]^h \tag{3.12}$$

$$f(x) = d\left(\frac{(ax+b)^{1/2} - c}{(ax+b)^{1/2} + c}\right)^h \tag{3.13}$$

and

$$f(x)=c\left(\frac{ax+b+1}{ax+b-1}\right)^{d}. \tag{3.14}$$

The transformation (3.14) contains the transformation (2.4) as a special case. Another special case is given by

$$g(x)=\tanh^{-1}\frac{(a+b)x-b}{(a-b)x+b}. \tag{3.15}$$

This transformation produces as a potential a well with a pole. The function (3.13) contains the transformation (2.39), which is used for symmetric potentials.

A special case of (3.12) is given by

$$g(x)=\tanh^{-1}\frac{\mathrm{i}}{2}\frac{1-2x}{[x(1-x)]^{1/2}}. \tag{3.16}$$

This transformation leads to a potential well with a barrier.

4. Potential well with a barrier

4.1. Solution of the Schrödinger equation

In this section the Schrödinger equation is solved completely and exactly with a potential, which is a special case of (3.7). The eigenvalues are determined explicitly and an expression in closed form is derived for all eigenfunctions. The method of solution is similar to that described in section 2. As an example, the potential well with a barrier is chosen that is derived from the potential (3.7) by the transformation (3.16),

$$U(z)=\hat{v}\left(\hat{q}_2\tanh^2 z+\hat{q}_1\frac{\tanh z}{\cosh z}+\hat{q}_0\right) \tag{4.1}$$

where

$$\hat{v}=\frac{2m\,\mathrm{d}^2}{\hbar^2}U_0 \qquad \text{dimensionless potential depth.}$$

The $\hat{q}_j$ are parameters, which can be chosen at will. Three potentials with different $\hat{q}_j$ are plotted in figure 1.

The potential (4.1) is considered, because, on the one hand, it is simple so that the Schrödinger equation can be solved with a relatively small expense of calculation. On the other hand, it is not known that there are exact solutions of the Schrödinger equation with similar potentials. Furthermore, the potential (4.1) contains the solved symmetric well (2.2) for $\hat{q}_1=0$ as a special case.

The dimensionless Schrödinger equation

$$\frac{\mathrm{d}^2\varphi}{\mathrm{d}z^2}+\left[\varepsilon-\hat{v}\left(\hat{q}_2\tanh^2 z+\hat{q}_1\frac{\tanh z}{\cosh z}+\hat{q}_0\right)\right]\varphi(z)=0 \tag{4.2}$$

is transformed by (3.16)

$$z=\tanh^{-1}\frac{\mathrm{i}}{2}\frac{1-2u}{[u(1-u)]^{1/2}}=\sinh^{-1}\mathrm{i}(1-2u) \tag{4.3}$$

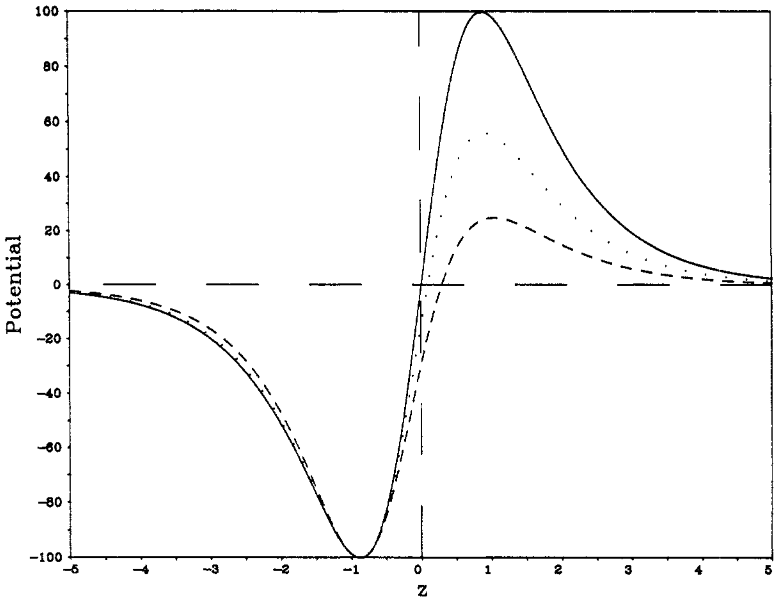

Figure 1. Potential well with a barrier. The three potentials, having different $\hat{q}_j$ values, are: —— $200 \tanh z/\cosh z$; ····· $43.69 \tanh^2(z+0.2)+150[\tanh(z+0.2)/\cosh(z+0.2)]-43.69$; ---- $74.91 \tanh^2(z+0.4)+100[\tanh(z+0.4)/\cosh(z+0.4)]-74.91$.

into the hypergeometric differential equation. Its normal form is

$$u^2(1-u)^2\frac{\mathrm{d}^2\Phi}{\mathrm{d}u^2}+\{[\varepsilon+\tfrac{1}{4}-\hat{v}(\hat{q}_2+\hat{q}_0)]u^2-[\varepsilon+\tfrac{1}{4}-\hat{v}(\hat{q}_2-\tfrac{1}{2}\mathrm{i}\hat{q}_1+\hat{q}_0)]u$$
$$+\tfrac{3}{16}-\tfrac{1}{4}\hat{v}(\hat{q}_2-\mathrm{i}\hat{q}_1)\}\Phi(u)=0. \tag{4.4}$$

This corresponds to the generally transformed differential equation (2.5). Thereby the real axis is mapped into a parallel of the imaginary axis through the point $\frac{1}{2}$:

$$\begin{aligned} &u=\tfrac{1}{2}(1+\mathrm{i}\sinh z)=\tfrac{1}{2}(1+\mathrm{i}x)\\ &x=\sinh z \qquad x\in[-\infty,+\infty]. \end{aligned} \tag{4.5}$$

The differential equation (4.4) is transformed using a result in [4]

$$\Phi(u)=u^{\lambda_1}(1-u)^{\lambda_2}y(u) \tag{4.6}$$

whereby

$$\begin{aligned} \lambda_1&=\tfrac{1}{2}+\tfrac{1}{2}[\tfrac{1}{4}+\hat{v}(\hat{q}_2-\mathrm{i}\hat{q}_1)]^{1/2}\\ \lambda_2&=\tfrac{1}{2}+\tfrac{1}{2}[\tfrac{1}{4}+\hat{v}(\hat{q}_2+\mathrm{i}\hat{q}_1)]^{1/2} \end{aligned} \tag{4.7}$$

into the hypergeometric differential equation

$$u(1-u)\frac{\mathrm{d}^2y}{\mathrm{d}u^2}+[-2(\lambda_1+\lambda_2)u+2\lambda_1]\frac{\mathrm{d}y}{\mathrm{d}u}+[-2\lambda_1\lambda_2-\varepsilon+\tfrac{1}{8}+\hat{v}(\tfrac{1}{2}\hat{q}_2+\hat{q}_0)]y(u)=0. \tag{4.8}$$

The transformation (4.6) prepares, like (2.8), the series expansion. Of course, the exponents are different on account of the different transformations (4.3) and (2.4). The differential equation (4.8) corresponds to (2.10). The solution of (4.8) is well known.

To determine the eigenvalues, the boundary conditions have to be applied to the solution of (4.8) later on. Therefore, the solution of (4.8) is expanded about $u = \infty$. The general solution of (4.8) is given by [5]

$$\begin{aligned} \varphi(z) = u^{\lambda_1 - 1/4}(1-u)^{\lambda_2 - 1/4}[&c_1 u^{-\alpha} F(\alpha, \alpha - \gamma + 1; \alpha - \beta + 1; u^{-1}) \\ &+ c_2 u^{-\beta} F(\beta, \beta - \gamma + 1; \beta - \alpha + 1; u^{-1})] \end{aligned} \tag{4.9}$$

$$u = \tfrac{1}{2}(1 + \mathrm{i}x) \qquad x = \sinh z \qquad |x| > \sqrt{3}$$

whereby

$$\begin{aligned} \alpha &= \lambda_1 + \lambda_2 - \tfrac{1}{2} + w \\ \beta &= \lambda_1 + \lambda_2 - \tfrac{1}{2} - w \\ \gamma &= 2\lambda_1 \\ w &= [\lambda_1^2 + \lambda_2^2 - \lambda_1 - \lambda_2 - \varepsilon + \tfrac{3}{8} + \hat{v}(\tfrac{1}{2}\hat{q}_2 + \hat{q}_0)]^{1/2}. \end{aligned} \tag{4.10}$$

4.2. Eigenvalues

The eigenvalues can be calculated from the general solution of the Schrödinger equation (4.9). They follow from the requirement that the solution (4.9) has to vanish at infinity and has to be finite in the whole range of definition. The boundary conditions cause one of the two linearly independent solutions of (4.9) to be resolved. The requirement of the finiteness in the range of definition results in the eigenvalue condition. Since the coefficients in the formula of the analytic continuation of the hypergeometric series are known, the eigenvalue condition can be given explicitly. Moreover, it can easily be solved for the eigenvalue.

At first the boundary condition at $z = -\infty$ ($x = -\infty$) is applied. The series in (4.9) take on the value one at the centre of the expansion. The complex powers of u have to be calculated only to derive the asymptotic representation

$$\begin{aligned} &\varphi(z) \to c_1 \sqrt{(1+x^2)}^{-\sqrt{[\hat{v}(\hat{q}_2 + \hat{q}_0) - \varepsilon]}} + c_2 \sqrt{(1+x^2)}^{\sqrt{[\hat{v}(\hat{q}_2 + \hat{q}_0) - \varepsilon]}} \\ &z \to -\infty \qquad x \to -\infty. \end{aligned} \tag{4.11}$$

The second term diverges so that

$$c_2 = 0. \tag{4.12}$$

As in the general case (2.26), one of the linearly independent solutions in (4.9) is resolved.

The range of definition of the series in (4.9) also contains $z = +\infty$ in addition to $z = -\infty$. Therefore, the second boundary condition at $z = +\infty$ is automatically satisfied, if (4.12) holds.

Now the finiteness of the solution (4.9) in the whole range of definition is required. The series in (4.9) are convergent, if $|x| > \sqrt{3}$. To study the wavefunction in the interval $x \in [-\sqrt{3}, \sqrt{3}]$, the remaining series in (4.9) has to be continued to this interval [5]. The analytic continuation is

$$\begin{aligned} \varphi(z) = (-1)^{\alpha} c_1 u^{\lambda_1 - 1/4}(1-u)^{\lambda_2 - 1/4}[&A F(\alpha, \beta; \gamma; u) \\ &- B u^{1-\gamma} F(\alpha - \gamma + 1, \beta - \gamma + 1; 2 - \gamma; u)] \end{aligned} \tag{4.13}$$

$$u = \tfrac{1}{2}(1 + \mathrm{i}x) \qquad x = \sinh z \qquad x \in \,]-\sqrt{3}, \sqrt{3}[$$

whereby

$$A=\frac{\Gamma(1-\gamma)\Gamma(\alpha-\beta+1)}{\Gamma(1-\beta)\Gamma(\alpha-\gamma+1)} \tag{4.14}$$

$$B=\mathrm{e}^{\mathrm{i}\pi(\gamma-1)}\frac{\Gamma(\gamma)\Gamma(1-\gamma)\Gamma(\alpha-\beta+1)}{\Gamma(2-\gamma)\Gamma(\gamma-\beta)\Gamma(\alpha)}. \tag{4.15}$$

Equation (4.13) corresponds to (2.31). A and B are the coefficients in the formula of the analytic continuation. The wavefunction (4.13) is convergent in the open interval $]-\sqrt{3},\sqrt{3}[$. At the points $x=\pm\sqrt{3}$ the series diverge. In order that φ is finite at these points, A and B have to vanish or the series have to terminate. The discussion of all possibilities results in the statement that it is sufficient, if either A or B vanishes. In this case the remaining series in (4.13) terminates so that the wavefunction is finite. A or B can vanish only if an argument of a Γ function in the denominator is equal to a negative integer. All possibilities result in the same eigenvalue condition

$$1-\beta=-n \qquad n\in\mathbb{N}_0. \tag{4.16}$$

If β is substituted by the help of (4.10), (4.16) can be solved for the eigenvalue

$$\varepsilon_n=\hat{v}(\hat{q}_2+\hat{q}_0)-[\![n+\tfrac{1}{2}-\{\tfrac{1}{2}[(\tfrac{1}{4}+\hat{v}\hat{q}_2)^2+\hat{v}^2\hat{q}_1^2]^{1/2}+\tfrac{1}{2}(\tfrac{1}{4}+\hat{v}\hat{q}_2)\}^{1/2}]\!]^2. \tag{4.17}$$

This is remarkable, since it is not possible for comparatively simple potentials (e.g., a square well).

From (4.16) and (4.17) it also follows that the spectrum is finite. The upper bound of the quantum number n is given by

$$n\leqslant\{\tfrac{1}{2}[(\tfrac{1}{4}+\hat{v}\hat{q}_2)^2+\hat{v}^2\hat{q}_1^2]^{1/2}+\tfrac{1}{2}(\tfrac{1}{4}+\hat{v}\hat{q}_2)\}^{1/2}-\tfrac{1}{2}. \tag{4.18}$$

4.3. *Eigenfunctions*

By the help of the eigenvalues (4.17) the eigenfunctions can be determined from the general solution of the Schrödinger equation (4.9). To do this the eigenvalue condition is substituted in the general solution. The result is that the hypergeometric series terminates. The eigenfunctions become Jacobi polynomials multiplied by powers of u in the whole range of definition, that is to say they are given in closed form.

The eigenfunctions follow from (4.9) and (4.12)

$$\varphi_n(z)=c_1u^{\lambda_1-1/4}(1-u)^{\lambda_2-1/4}u^{-\alpha}F(\alpha,\alpha-\gamma+1;\alpha-\beta+1;u^{-1}). \tag{4.19}$$

The hypergeometric series can be transformed into [5]

$$\varphi_n(z)=c_1u^{\lambda_1-1/4}(1-u)^{\lambda_2-1/4}u^{\beta-\gamma}(u-1)^{\gamma-\alpha-\beta}F(1-\beta,\gamma-\beta;\alpha-\beta+1;u^{-1}). \tag{4.20}$$

By the help of the eigenvalue condition (4.16), the first parameter of the series (4.20) becomes a negative integer. Therefore the series terminates and turns into a polynomial of nth degree.

Completely analogously the expression

$$\varphi_n(z)=-(-1)^{\alpha}c_1u^{\lambda_1-1/4}(1-u)^{\lambda_2-1/4}Bu^{1-\gamma}(1-u)^{\gamma-\alpha-\beta}F(1-\beta,1-\alpha;2-\gamma;u) \tag{4.21}$$

follows from (4.13). Since this series also terminates, the division of the intervals in (4.9) and (4.13) is superfluous. Therefore (4.20) and (4.21) have to be identical. This can be proved by substituting the series representation of the hypergeometric functions in these expressions.

The terminating hypergeometric series can be expressed by Jacobi polynomials. By the help of (4.10) and (4.16), the eigenfunctions are of the form

$$\varphi_n(z) = c_1(-1)^{4\lambda_1+2\lambda_2+1}\frac{n!}{(2\lambda_1+2\lambda_2-n-2)_n}$$
$$\times u^{-\lambda_1+3/4}(1-u)^{-\lambda_2+3/4}P_n^{(-2\lambda_1+1;-2\lambda_2+1)}(-\mathrm{i}\sinh z) \qquad (4.22)$$

$u=\frac{1}{2}(1+\mathrm{i}\sinh z)$.

It is obvious that the expression (4.22) is complex. It can be proved, however, that the part which depends on the spatial coordinate, is real. A representation, which expresses this property, is not as compact as (4.22).

4.4. Comparison with the simple potential well

The simple symmetric well (2.2) is a special case of the potential well with a barrier (4.1). It is interesting to compare the discrete spectra of both potentials.

From (4.17) it follows that the spectra of the well with a barrier and of the simple symmetric well are of the same mathematical form;

$$\varepsilon_n = a_0-(n+a_1)^2. \qquad (4.23)$$

The a_j are functions of the potential parameters. Since (4.23) holds for both potentials, there exists for each well with a barrier exactly one simple symmetric well, which has exactly the same spectrum. The number of eigenvalues is the same and their absolute values are identical. It is remarkable that this result is independent of the number of eigenvalues. The potential parameters q_j of the simple well can be calculated from the

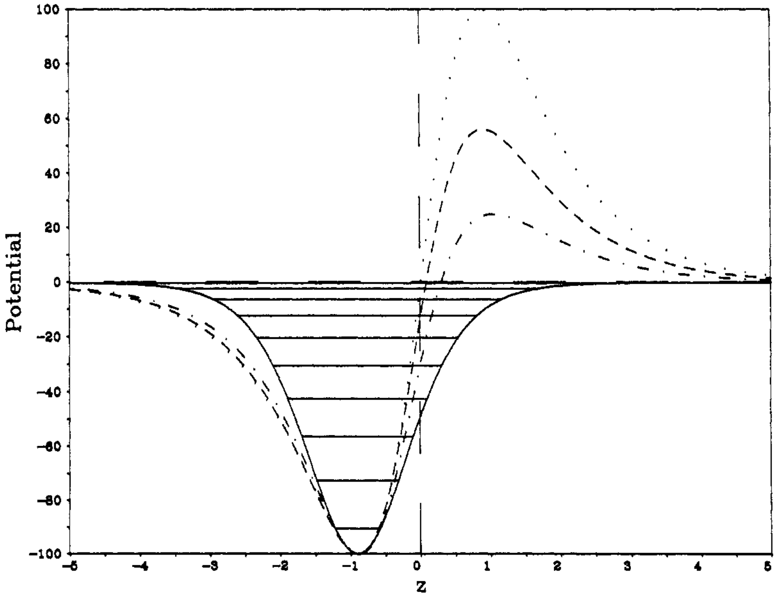

Figure 2. Eigenvalues of the potential well with a barrier. The four potentials are: —— $99.88\tanh^2(z+0.9)-99.88$; ····· $200\tanh z/\cosh z$; ---- $43.69\tanh^2(z+0.2)+150[\tanh(z+0.2)/\cosh(z+0.2)]-43.69$; -·-·- $74.91\tanh^2(z+0.4)+100[\tanh(z+0.4)/\cosh(z+0.4)]-74.91$.

parameters of the well with a barrier $\hat{q}_j$. They are connected by

$$\begin{aligned} vq_2 &= \tfrac{1}{2}\{[(\tfrac{1}{4}+\hat{v}\hat{q}_2)^2+\hat{v}^2\hat{q}_1^2]^{1/2}+\hat{v}\hat{q}_2-\tfrac{1}{4}\} \\ vq_1 &= 0 \\ vq_0 &= \hat{v}\hat{q}_0-\tfrac{1}{2}\{[(\tfrac{1}{4}+\hat{v}\hat{q}_2)^2+\hat{v}^2\hat{q}_1^2]^{1/2}-\hat{v}\hat{q}_2-\tfrac{1}{4}\}. \end{aligned} \tag{4.24}$$

Conversely there exists to each simple well a whole family of wells with a barrier, which have the same spectrum. This assignment is not single valued, because the well with a barrier provides three potential parameters to express the two parameters a_j in (4.23).

In figure 2 four potentials, which have the same eigenvalue spectrum, are plotted. The equivalence concerns the eigenvalues. The eigenfunctions of the potentials are, of course, different.

5. Conclusion

With the method described above, it is possible to solve the Schrödinger equation with the potential (3.7) exactly and analytically. From this it follows that all the calculations have to be worked out only once. This results in a great reduction of time compared with the numerical solution of the Schrödinger equation, especially if the potential has many eigenvalues or if the potential parameters are varied. In section 4.4 the equivalence of the spectra of two different potentials was proven. Such an assertion is completely impossible with numerical methods.

The well with a barrier is one of the simplest potentials that can be deduced from (3.7). The appropriate transformation contains only four arbitrary parameters. The most general transformation (3.9) has eight algebraic parameters. From the transformations, investigated up to now, it can be concluded that the complexity of the potentials increase with the number of parameters of the transformation. There is hope that the double-well potentials can also be solved by (3.9). A double well is present if the derivative of the potential has three finite real zeros. In fact some transformations produce equations of third degree for this expression. Since the parameters of the equation define the extrema of the potential as well as the range of definition, until now it could not be proved that it is possible to place all the zeros in the range of definition. Exact solutions of double-well potentials are particularly interesting. Completely new methods could be deduced from them, for example, for almost degenerate states.

If the degrees of the polynomials in (3.9) are fixed, the integration results in 23 transformations, which are similarly constructed like (3.10) to (3.14). The number of transformations can be increased, if the requirement (3.5) is dropped and if other differential equations are allowed. In particular, the Schrödinger equations derived by (3.9) can be used as solved differential equations in (3.5). Then new transformations can be derived. If this method is used several times, the number of transformations and that of the solved Schrödinger equations might become unlimited.

Finally, (3.7) contains potentials, which can be solved by the general method described in sections 2. The eigenvalues of these potentials are solutions of the general eigenvalue condition (2.35). On account of the generality of (2.35) and of the same form for different potentials it should be expected that these solutions can be generalised, so that (2.35) can be solved for the general potential (2.1).

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