Exact Solutions of the Schrödinger Equation

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In classical mechanics the problem of determining the forms of potential function which permit solution in terms of known functions received considerable attention. The present paper is a partial study of the same problem in quantum mechanics. A method is given for determining the forms of potential function which permit an exact solution of the one-dimensional Schrödinger equation in terms of series whose coefficients are related by either two or three term recursion formulas. The more interesting expressions for the potential energy have been tabulated. A correspondence is found between these solutions and the solutions of the corresponding Hamilton-Jacobi equation. It is shown that whenever the Hamilton-Jacobi equation is soluble in terms of circular or exponential functions, the corresponding Schrödinger equation is soluble in terms of a series whose coefficients are related by a two-term recursion formula. Whenever the Hamilton-Jacobi equation is soluble in terms of elliptic functions, the corresponding Schrödinger equation is soluble in terms of a series whose coefficients are related by a three-term recursion formula. For the first case the quantized values of the energy are found by restricting the series to a polynomial and in the second by finding the roots of a continued fraction. A brief discussion of the technique of solution of continued fractions is given.

Exact Solutions in Classical Mechanics

In either classical mechanics or in the Bohr-Sommerfeld formulation of quantum mechanics, the solution of a problem involves evaluation of an integral of the form:

$$\int [2m(E-V)(dr/dx)^2]^{\frac{1}{2}} dx \qquad (1)$$

where r is the coordinate and x is a function of r in terms of which the integration is simpler. If the integrand is expressed as a radical divided by a rational function of x, the degree of the expression under the radical determines the kind of function in terms of which the integral can be expressed. If the expression is quadratic in x, the integral can be solved in terms of circular functions; if the expression is of the third or fourth degree in x, the integral can be solved in terms of elliptic functions.

Exact Solutions in Quantum Mechanics

If rotation is neglected, the one-dimensional Schrödinger equation has the form,

$$d^2R/dr^2 + k[E-V(r)]R = 0, \qquad (2)$$

where $k=8\pi^2 mc/h$, E is the energy in cm^{-1}.

In order to obtain exact solutions of the differential equation for many interesting forms of potential functions, it is necessary to make a transformation of the independent variable. If the transformation $x=x(r/\rho)$ is carried out, the result is:

$$R'' + \left[\frac{d^2x/dr^2}{(dx/dr)^2}\right]R' + \left[\frac{W-\Phi}{\rho^2(dx/dr)^2}\right]R = 0, \qquad (3)$$

where $W=k\rho^2 E$, $\Phi = k\rho^2 V$.

If dx/dr has the form $x^{A_0}(1-x)^{-A_1}(a+x)^{A_2}$ the coefficient of R becomes $A_0/x + A_1/(1-x) + A_2/(a+x)$.

The coefficient of R is, except for a constant, the same as the expression under the radical in Eq. (1).

The problem of obtaining an exact solution of the one-dimensional Schrödinger equation requires the solution of a linear second order differential equation. The methods of solution of such an equation depend upon the number and character of the singular points of the differential equation. For the purposes of the present study, six types of equations will be considered. These six types are all special cases of a more general equation. This more general equation is:

$$R'' + \left[\frac{A_1}{1-x} + \frac{A_2}{a+x} + \frac{A_0}{x}\right]R' + \left[\frac{B_0}{x^2} + \frac{B_1}{(1-x)^2} + \frac{B_2}{(a+x)^2} + \frac{C_1 x + C_2}{x(1-x)(a+x)} + \frac{C_3}{x} + \frac{C_4}{1-x} - \mu^2 + C_6 + C_5 x - \epsilon^2 x^2 - \frac{\delta^2}{x^4} + \frac{B_3}{x^3}\right]R = 0, \qquad (4)$$

of which there is a solution of the form:

$$R = x^{\alpha}(1-x)^{\beta}(a+x)^{\gamma} e^{-\delta/x - \mu x - \epsilon x^2/2} \sum a_n x^n. \qquad (5)$$

TABLE I. *Classification of equations.*

Type	Constants of Eqs. (4) and (5) which are zero	Reg. sing. pts.	Irreg. sing. pts. 2nd species	Irreg. sing. pts. 4th species	Known examples
I	$A_2, B_2, C_2-C_1a, C_3, C_4, C_6, \mu, C_5, \epsilon, \delta, B_3, \gamma$	$0, +1, \infty$			Hypergeometric
II	$A_1, A_2, B_1, B_2, C_1, C_2, C_4, C_6, C_5, \epsilon, \delta, B_3, \beta, \gamma$	0	∞		Confl. hypergeometric
IIIa	$C_3, C_4, C_6, \mu, C_5, \epsilon, \delta, B_3$	$0, +1, a<-1, \infty$			Lamé
IIIb	" "	$0, +1, a>+1, \infty$			"
IVa	$A_2, B_2, C_1, C_2, C_6, C_5, \epsilon, \delta, B_3, \gamma$	$0, +1,$	∞		Spheroidal
IVb	" "	$0, -1,$	∞		"
V	$A_1, A_2, B_1, B_2, C_1, C_2, C_4, C_5+2\mu\epsilon, \delta, B_3, \beta, \gamma$	0		∞	
VI	$A_1, A_2, B_1, B_2, C_1, C_2, C_4, \beta, \gamma, C_6, C_5, \epsilon$		$0, \infty$		Mathieu

The above table gives the essential characteristics of the six types of equations. In the first column is the number by which that type of equation will be referred to; in the second column are listed the constants of Eqs. (4) and (5) which are zero for that type of equation; in the third column the regular singular points of the equation are listed; in the fourth column the irregular singular points of the second species[1] are listed, and in the fifth column the essential singular points of the fourth species[1] are listed. Many of these equations, or their special cases, have been studied and named. These names are given in the last column of Table I.

For the first two types of equation the recursion relation involves only two of the a_n's. For the other four types of equations the recursion involves three of the a_n's. For the first five types of equation, there will be two roots of the indicial equation, although it may be that only one of the roots gives a solution satisfying the boundary conditions. For the sixth type of equation, there will be at most only one root of the indicial equation.

Forms of Potential Functions Permitting an Exact Solution

From Eq. (3) it follows that if a differential equation of a given type is to be a transformed Schrödinger equation, one term in the coefficient of R must have the form of a constant divided by a function of x. If this constant is taken to be W and the denominator set equal to $\rho^2(dx/dr)^2$, a differential equation is obtained which can be solved for r as a function of x and by inversion for x as a function of r. The remaining terms in the coefficient of R are then taken to be $-\Phi/\rho^2(dx/dr)^2$. By this method Φ can be found as a function of r. A very large number of transformations can be found but for many of them x can be obtained from r only as a table of values. In the table which follows, consideration is limited to those transformations where x is defined as either a power of r or as an exponential function of r. In the adjoining table, the first column gives the type of differential equation considered, the second gives the constant which is taken to be W, the third gives the expression for $\rho dx/dr$, the fourth gives the expression for x as a function of r, the fifth column gives the expression for the potential energy, and the last column gives the reference for the cases that have been investigated.[2] For the sake of brevity, the various constants in the expression for Φ have been combined and the following substitutions used: $z=r/2\rho$, $u=1/x$, $v=1/1-x$, $w=1/1+x$, $s=1/a+x$.

The first list includes the cases for which valid solutions (for certain values of the energy) can be found in terms of convergent series about the origin. The second list includes those cases for which it may be necessary to join solutions about different singular points to obtain valid solutions. In any case the solutions for potential functions given in the second list must be examined in detail for each special case. For the potential functions which lead to Eq. III there

[1] For a discussion of the "species" of an irregular singular point, see Ince, *Ordinary Differential Equations*, Chap. 20.

[2] Essentially this method has been used by Rosen to determine the forms of potential function soluble in terms of hypergeometric or confluent hypergeometric functions. Since these results have not been published, they are included here for completeness.

TABLE II. *Potential functions permitting exact solutions.*

TYPE	W	$\rho dx/dr$	x	Φ	REFERENCES
I	B_0	$-x$	$\pm e^{-2z}$	$K_1x^2v^2+K_2xv$	1, 2, 3, 4
I	B_0	$x(1-x)^{\frac{1}{2}}$	$\text{sech}^2 z$	$K_1x+K_2x^2v$	5
II	$-\mu^2$	1	$2z$	$K_1u+K_2u^2$	6, 7
II	C_3	$x^{\frac{1}{2}}$	z^2	K_1u+K_2x	6, 8
II	B_0	$-x$	e^{-2z}	$K_1x+K_2x^2$	9
III	B_0	$-x$	$\pm e^{-2z}$	$K_1x^2v^2+K_2x^2s^2+(K_3x+K_4x^2)vs$	
III	B_0	$x(1-x)^{\frac{1}{2}}$	$\text{sech}^2 z$	$K_1x+K_2xs+K_3x^2v+K_4x^2(1-x)s^2$	
IVa	B_0	$-x$	$\pm e^{-2z}$	$K_1x+K_2x^2+K_3x^2v+K_4x^2v^2$	
IVa	B_0	$x(1-x)^{\frac{1}{2}}$	$\text{sech}^2 z$	$K_1x+K_2x^2+K_3x^3+K_4v$	10
V	C_3	$x^{\frac{1}{2}}$	z^2	$K_1u+K_2x+K_3x^2+K_4x^3$	11
V	B_0	$-x$	e^{-2z}	$K_1x+K_2x^2+K_3x^3+K_4x^4$	
V	C_5	$x^{-\frac{1}{2}}$	$(3z)^{\frac{2}{3}}$	$K_1u^3+K_2u^2+K_3u+K_4x$	
V	$-\epsilon^2$	$1/x$	$2z^{\frac{1}{2}}$	$K_1u^4+K_2u^3+K_3u^2+K_4u$	
V	B_3	1	$2z$	$K_1u^2+K_2u+K_3x+K_4x^2$	
IVa	$-\mu^2$	± 1	$\pm 2z$	$K_1u^2+K_2u+K_3v+K_4v^2$	
IVa	C_3	$x^{\frac{1}{2}}$	$\pm z^2$	$K_1u+K_2x+K_3xv+K_4xv^2$	
IVb	C_3	$(x(1+x))^{\frac{1}{2}}$	$\sinh^2 z$	$K_1x+K_2x^2+K_3xw+K_4u$	
VI	B_2	$-x$	e^{-2z}	$K_1u^2+K_2u+K_3x+K_4x^2$	
VI	C_3	$x^{\frac{1}{2}}$	z^2	$K_1u^3+K_2u^2+K_3u+K_4x$	
VI	$-\mu^2$	1	$2z$	$K_1u^4+K_2u^3+K_3u^2+K_4u$	

[1] Eckart, Phys. Rev. **35**, 1303 (1930).
[2] Rosen and Morse, Phys. Rev. **42**, 210 (1932).
[3] Manning and Rosen, Phys. Rev. **44**, 953 (1933).
[4] Newing, Phil. Mag. **19**, 759 (1935).
[5] Poeschl and Teller, Zeits. f. Physik **83**, 143 (1933).
[6] Schrödinger, Ann. d. Physik **76**, 361 (1926).
[7] Shortley, Phys. Rev. **38**, 120 (1931).
[8] Davidson, Proc. Roy. Soc. **A135**, 459 (1932).
[9] Morse, Phys. Rev. **34**, 57 (1929).
[10] Manning, J. Chem. Phys. **3**, 136 (1935).
[11] Morse and Stückelberg, Helv. Phys. Acta **4**, 337 (1931).

will also be the cases when a is replaced by $-a$ and the case when $a=-1$. For the case $a=-1$ there is a possible transformation $x=\text{sech}\ 2z$ for which the corresponding potential function belongs in the second group.

If, in Eqs. I and II, the coefficient of R is written over a common denominator, the numerator is quadratic in x. By comparison of Eqs. (1) and (3), it follows that whenever the Hamilton-Jacobi equation is soluble in terms of circular functions,[3] the corresponding Schrödinger equation is soluble in terms of functions characterized by a two term recursion relation. If in Eqs. III, IV, V, VI, the coefficient of R is written over a common denominator, the numerator will be of the fourth degree in x. Hence, it follows that whenever the Hamilton-Jacobi equation is soluble in terms of elliptic functions,[3] the corresponding Schrödinger equation is soluble in terms of functions characterized by a three-term recursion relation.

[3] In accordance with what has been said, it follows that the classical solutions for the potential functions listed here can be found in terms of either circular or elliptic functions. The transformations of the form $x=r^n$ are discussed in the fourth chapter of Whittaker's *Analytical Dynamics*, but the other transformations have received little attention in textbooks on classical mechanics.

BOUNDARY CONDITIONS AND METHOD OF DETERMINING ENERGY LEVELS

The solutions for all forms of potential function which lead to differential equations of the first two types have been given in the literature. It turns out that, for these cases, whenever the total energy is less than the potential energy at both plus and minus infinity, solutions satisfying the boundary conditions can be found only for those values of the energy for which the infinite series reduces to a polynomial.

For the last four types of equation, the recursion relation between coefficients has the form

$$H_n b_{n+1} + 1 + M_n/b_n = 0, \qquad (6)$$

where $b_n = a_n/a_{n-1}$ and H_n and M_n are expressible in terms of the various constants and the running number n. The convergence of such a series can be tested by a method given by MacLaurin.[4] The essential feature of this method is the assumption (which can be justified) that at large n, $b_{n+1}=b_n[1+0(1/n)]$. When this substitution is made, Eq. (6) reduces to a quadratic equation which can be solved for b_n. If one of the roots of this equation satisfies the ordinary convergence test, a series solution satisfying

[4] MacLaurin, Trans. Camb. Phil. Soc. **17**, 33 (1898).

the boundary conditions can be found for certain values of the energy. For Eq. III, Eq. IV when the range of the variable to from zero to unity, and Eq. V the necessary conditions are fulfilled. For Eq. VI and Eq. IV when the range of the variable includes infinity, the series will converge in only a restricted region and it is necessary to use some method of joining solutions which are valid about different expansion points.

The series solution must satisfy two conditions. There must be no terms containing negative powers of x, and at large n the ratio of two successive coefficients must approach the allowed limiting value found by the method just described. If Eq. (6) is written for $n=0$, the first condition causes this relation to reduce to:

$$0=1+H_0 b_1. \tag{7}$$

By using Eq. (16) to solve for b_1 in terms of H_1, M_1 and b_2 and then to find b_2 in terms of succeeding values of H, M and b, the result is

$$0=1-\frac{Q_0}{1-\dfrac{Q_1}{1-\dfrac{Q_2}{1\cdots\dfrac{Q_{l-1}}{1-H_l b_{l+1}}}}} \tag{8}$$

where $Q_n=H_n M_{n+1}$.

At sufficiently large n the asymptotic value of b_n can be substituted without appreciable error, and the continued fraction terminated. For a given set of constants in the potential function and an arbitrary value of the energy, the result found by carrying out the process of repeated divisions and subtractions will not be zero but will be a function of the value assumed for the energy. This function will be zero only for certain values of the energy—these are the values of the energy for which the boundary conditions are fulfilled. The problem of determining these values must, except for the simplest cases, be carried out numerically. The method used is similar to that used in finding the roots of an algebraic equation of degree higher than the fourth and consists of evaluating the left-hand side of Eq. (8) for two values of W and interpolating or extrapolating for a better approximation to the value of W which makes the left-hand side of Eq. (8) vanish. The process can be repeated until the desired accuracy is reached. The value of the continued fraction as a function of the value of W has a number of branches and when extrapolating or interpolating care must be taken that the points used are all on the same branch.

The form given in (8) is not always satisfactory for numerical solution. By repeated inversions (8) can be transformed into

$$\frac{Q_m}{1-\dfrac{Q_{m+1}}{1-\dfrac{Q_{m+2}}{1\cdots}}}=1-\frac{Q_{m-1}}{1-\dfrac{Q_{m-2}}{1-\cdots\dfrac{Q_1}{1-Q_0}}}. \tag{9}$$

The values of the energy which make these two expressions equal are the ones for which the boundary conditions are satisfied. The best form of Eq. (9) for numerical solution is when Q_m in the numerator of the left-hand side is the largest of all the Q's.

For Eq. VI it is necessary to expand about an essential singular point. Detailed examination shows that the boundary conditions at $x=0$ can be satisfied only by so choosing the root (there is only one) of the indicial equation that there are at most only a finite number of negative powers of x in the series expansion. The series so found will converge for finite values of x but will diverge at x equal infinity. If a similar series expansion about x equal infinity is found it will have the same properties in terms of $1/x$.

By properly choosing the scale factor ρ the continued fraction corresponding to the solution valid about x equal infinity can be made the same as the continued fraction corresponding to the solution valid about x equal zero. For the values of the energy obtained by solution of this continued fraction it will be possible to join the two solutions at some intermediate point (say x equal unity) and thus obtain solutions valid throughout the entire range of the independent variable. It may be pointed out that this method is somewhat similar to that used for the Mathieu equation which is a special case of Eq. VI.

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