Matematisk-fysiske Meddelelser
udgivet af
Det Kongelige Danske Videnskabernes Selskab
Bind **32**, nr. 4

Mat. Fys. Medd. Dan. Vid. Selsk. **32**, no. 4 (1960)

ON THE SCHRÖDINGER EIGENVALUE PROBLEM

BY

OLAVI HELLMAN

København 1960
i kommission hos Ejnar Munksgaard

CONTENTS

Synopsis

The Schrödinger eigenvalue problem is treated by a matrix method. A procedure for obtaining eigenvalues is developed for the following rather general cases: 1) $l = 0$, and the potential function is assumed to be integrable in the Lebesgue sense over a finite interval $(0, L)$, vanishing elsewhere; 2) $l \neq 0$, and the potential is assumed to be of the form $\frac{a}{r^2} - \frac{b}{r} + V_0(r)$, $V_0(r)$ possessing a power-series expansion within the interval $(0, L)$ and vanishing elsewhere (this expansion will not, however, be needed in the calculations). The eigenvalues appear as roots of a rapidly converging power series. The eigenfunctions are expressed directly in terms of the functions obtained in the process of forming the above power series.

Printed in Denmark
Bianco Lunos Bogtrykkeri A-S

1. Introduction

In the present paper we are going to consider the SCHRÖDINGER eigenvalue problem

$$\left.\begin{aligned} &\frac{d^2R}{dr^2}+\frac{2}{r}\frac{dR}{dr}-\frac{l(l+1)}{r^2}R+k(\lambda-V(r))R=0\\ &R(0)<\infty \quad \text{and} \quad R(r)\to 0, \quad \text{as} \quad r\to\infty \end{aligned}\right\} \tag{1.1}$$

in the following two—fairly general—cases:

CASE I: $l=0$, and the potential $V(r)$ differs from zero only within a finite interval $[0, L]$. Besides that, we only assume that $V(r)$ is integrable in the Lebesgue sense over the interval $[0, L]$. By doing this we believe to have included all potential functions of practical interest with the sole restriction that the possible singularities of the potential function for some $r' \varepsilon [0, L]$ must be of the order $(r-r')^{-\alpha}$, where $\alpha<1$.

CASE II: $l \neq 0$, and the potential is of the form

$$V(r)=\frac{a}{r^2}-\frac{b}{r}-V_0(r), \tag{1.1 a}$$

where necessarily $a\neq 0$ (more precisely: $\sqrt{(2l+1)^2+4ka}$ must not be an integer). Furthermore, $V_0(r)$ is assumed to be different from zero only within the interval $[0, L]$, possessing there an absolutely convergent power-series expansion. This expansion will not, however, be needed in the calculations.

The basic idea of our considerations is the following: we throw the differential equation (1.1) into the matrix form

$$\frac{d}{dr}\begin{pmatrix}R'\\R\end{pmatrix}-\begin{pmatrix}-\frac{2}{r} & \frac{l(l+1)}{r^2}+k(\lambda-V(r))\\ 1 & 0\end{pmatrix}\begin{pmatrix}R'\\R\end{pmatrix}=0 \tag{1.2}$$

and are thus led to consider a matrix differential equation of the first order, to which many useful mathematical relations apply.

Let us write (1.2) more briefly as

$$\frac{dz}{dr} - B(r)\, z = 0, \tag{1.2 a}$$

where z and $B(r)$ are clear from (1.2).

In *CASE I* it is easy to find a matrix $D(r)$ such that the transformation $z = D\eta$ leads to a matrix differential equation

$$\frac{d\eta}{dr} - A(r)\, \eta = 0 \tag{1.2 b}$$

in which the elements of $B(r)$ are functions integrable in the Lebesgue sense over the interval $[0, L]$. If we now require that $\eta(0) = \eta_0$, then the unique solution of (1.2 b) will be the well-known matrix series

$$\eta = \left(I + \int_0^r A dr + \int_0^r A dr_1 \int_0^{r_1} A dr_2 + \ldots \right) \eta_0 = \Omega_0^r(A)\, \eta_0, \tag{1.3}$$

where I denotes the unit matrix. The matrix $\Omega_0^r(A)$ is usually called a matrizant. The properties of the matrizant will be discussed in section 2.

The conditions which were imposed upon $R(r)$ are now written into matrix form, and finally—as will be shown in section 2—the formula

$$\det \left\{ \Omega_0^L(A) \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{matrix} -\sqrt{k\,|\lambda|} \\ 1 \end{matrix} \right\} = 0 \tag{1.4}$$

for the eigenvalues is obtained.

As we see from (1.4), the matrizant $\Omega_0^L(A)$ is the core of our eigenvalue problem.

The forming of $\Omega_0^r(A)$ is possible, but highly unpractical to carry out by means of the definition (1.3). In section 3 a procedure is developed which, avoiding the direct use of (1.3), gives the matrizant $\Omega_0^r(A)$ as a power series in λ. This procedure is very little sensitive to the form of the potential function; only the above-mentioned Lebesgue integrability is needed to assure the convergence of the series obtained. The procedure is particularly well suited for handling eigenvalue problems where the potential is given in tabular form. The left-hand side of (1.4) becomes an infinite convergent power series in $\sqrt{k|\lambda|}$ whose real zero points—when such points exist—are the discrete eigenvalues of our problem. As an application, the case of a square well is considered in section 3.

In *CASE II*, where $l \neq 0$ and where the potential function is of the form (1.1 a), it is impossible to find a matrix $D(r)$ such that the transformation $z = D(r)\eta$ leads from the differential equation (1.2 a) to a differential equation (1.2 b) in which the elements of $A(r)$ are functions integrable in the Lebesgue sense. The simplest form which one may obtain from (1.2 a) in this manner turns out to be

$$\frac{d\eta}{dr} - \left(\frac{C}{r} + G(r)\right)\eta = 0, \tag{1.5}$$

where C is a constant matrix and where $G(r)$ has the same properties as $A(r)$ in (1.2 a). As is well known, the matrizant (1.3) does not exist for the matrix $\frac{C}{r} + G(r)$. It is possible, however, to obtain—by application of well-known theorems from the matrix calculus—a matrizant-like solution of (1.5), as is shown in section 5. Also a procedure of giving this modified matrizant as a power series in λ is developed there.

The eigenvalue equation for *CASE II* is derived in section 4. The formula obtained is very similar to the formula (1.4). It contains, besides the modified matrizant, Whittaker functions. The eigenvalue problem of *CASE II* is somewhat more complicated than that of *CASE I*. There is, however, no essential difference in the handling of the two cases.

In both the above cases the functions we obtain when forming the matrizant yield the eigenfunctions without further calculations.

2. *Case I*

We shall consider the eigenvalue problem

$$\left.\begin{aligned} &\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} - k(|\lambda| + V(r))\,R = 0 \\ &R(0) < \infty \quad \text{and} \quad R(r) \to 0, \ \text{as} \ r \to \infty \end{aligned}\right\} \tag{2.1}$$

arising from (1.1) when we put $l = 0$. Here $|\lambda|$ denotes the absolute value of the negative eigenvalue λ. The potential function $V(r)$ has the properties given on page 3.

The substitution

$$R = \frac{w}{r} \tag{2.2}$$

brings (2.1) into the form

$$\left.\begin{aligned} \frac{d^2 w}{dr^2} - k(|\lambda| + V(r))\, w = 0 \\ w(r) = 0(r^v),\ v \geqslant 1, \quad \text{as} \quad r \to 0, \quad \text{and} \quad w(r) \to 0, \quad \text{as} \quad r \to \infty. \end{aligned}\right\} \tag{2.3}$$

We now throw the eigenvalue problem (2.3) into matrix form as follows:

$$\left.\begin{aligned} \frac{d}{dr}\begin{pmatrix} \dfrac{dw}{dr} \\ w \end{pmatrix} - \begin{pmatrix} 0 & k(|\lambda| + V(r)) \\ 1 & 0 \end{pmatrix}\begin{pmatrix} \dfrac{dw}{dr} \\ w \end{pmatrix} = 0 \\ \begin{pmatrix} \dfrac{dw}{dr} \\ w \end{pmatrix}_{r=0} = C_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \dfrac{dw}{dr} \\ w \end{pmatrix} \to \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \text{ as } r \to \infty, \end{aligned}\right\} \tag{2.4}$$

where C_1 is a real constant. At $r = 0$, the above is a necessary condition for $w(r) = 0(r^v)$, $v \geqslant 1$. It is, however, also sufficient, as will be seen later (cf. (2.15)).

The differential equation in (2.4) is of the form

$$\frac{dz}{dr} - Az = 0, \tag{2.5}$$

where, in our case,

$$z = \begin{pmatrix} \dfrac{dw}{dr} \\ w \end{pmatrix} \quad \text{and} \quad A = \begin{pmatrix} 0 & k(|\lambda| + V_0(r)) \\ 1 & 0 \end{pmatrix}.$$

If it is required that $z(0) = z_0$ (= const.), the unique solution of (2.5) will be, according to what was said in section 1, the series

$$z(r) = \left(I + \int_0^r A\, d\tau_1 + \int_0^r A\, d\tau_1 \int_0^{\tau_1} A\, d\tau_2 + \dots\right) z_0 = \Omega_0^r(A)\, z_0, \tag{2.6}$$

where I is the unit matrix.

For our present purpose we mention the following facts about the matrizant (1):

Let the elements $A_{ij}(r)$ of A be functions integrable in the Lebesgue sense in the finite interval $[0, L]$. Then

1° the series (2.6) converges absolutely and uniformly in $[0, L]$,
2° the inverse of $\Omega_0^r(A)$ exists for every $r \varepsilon [0, L]$,
3° $\Omega_0^r(A+B) = \Omega_0^r(A)\, \Omega_0^r\{[\Omega_0^r(A)]^{-1} B\, \Omega_0^r(A)\}$,
4° for a constant matrix A we shall have $\Omega_0^r(A) = \exp(Ar)$,
5° $\det \Omega_0^r(A) = \exp\left(\int_0^r Tr\, A\, d\tau\right)$.

We now return to the eigenvalue problem (2.4). Let us write

$$A_I = \begin{pmatrix} 0 & k(|\lambda| + V(r)) \\ 1 & 0 \end{pmatrix}$$

$$A_{II} = \begin{pmatrix} 0 & k|\lambda| \\ 1 & 0 \end{pmatrix}$$

$$w(r) = \begin{cases} w_I\ (r) & \text{for } r\,\varepsilon\,[0, L] \\ w_{II}(r) & \text{for } r\,\varepsilon\,[L, \infty]. \end{cases}$$

Then, according to what was said above,

$$\begin{pmatrix} \dfrac{dw_I}{dr} \\ w_I \end{pmatrix} = \Omega_0^r(A_I) \begin{pmatrix} C_1 \\ 0 \end{pmatrix} \tag{2.7}$$

and

$$\begin{pmatrix} \dfrac{dw_{II}}{dr} \\ w_{II} \end{pmatrix} = \Omega_0^r(A_{II})\, z_{II}, \tag{2.8}$$

where z_{II} is a constant vector. Since A_{II} is a constant matrix, we have (according to the property 4° of the matrizant)

$$\Omega_0^r(A_{II}) = \exp\left[\begin{pmatrix} 0 & k|\lambda| \\ 1 & 0 \end{pmatrix} r\right]. \tag{2.9}$$

This may be rewritten by the aid of the Sylvester expansion as follows:

$$\exp\left[\begin{pmatrix}0 & k|\lambda| \\ 1 & 0\end{pmatrix} r\right] = \exp\left(\sqrt{k|\lambda|}\, r\right) \mathfrak{L}_1 + \exp\left(-\sqrt{k|\lambda|}\, r\right) \mathfrak{L}_2, \tag{2.9a}$$

where

$$\mathfrak{L}_1 = \frac{1}{2}\begin{pmatrix} 1 & \sqrt{k|\lambda|} \\ \dfrac{1}{\sqrt{k|\lambda|}} & 1 \end{pmatrix} \tag{2.10}$$

and

$$\mathfrak{L}_2 = \frac{1}{2}\begin{pmatrix} 1 & -\sqrt{k|\lambda|} \\ -\dfrac{1}{\sqrt{k|\lambda|}} & 1 \end{pmatrix}. \tag{2.11}$$

Since we require in (2.4) that

$$\begin{pmatrix} \dfrac{dw_{II}}{dr} \\ w_{II} \end{pmatrix} \to \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad \text{as} \quad r \to \infty,$$

the vector z_{II} in (2.8) must be chosen so that $\mathfrak{L}_1 z_{II} = 0$, i. e.,

$$z_{II} = \begin{pmatrix} -\sqrt{k|\lambda|} \\ 1 \end{pmatrix} C_2, \tag{2.12}$$

C_2 being a real constant. We then have

$$\begin{pmatrix} \dfrac{dw_{II}}{dr} \\ w_{II} \end{pmatrix} = e^{-\sqrt{k|\lambda|}\, r} \begin{pmatrix} -\sqrt{k|\lambda|} \\ 1 \end{pmatrix} C_2. \tag{2.8a}$$

It is now required that the vectors $\begin{pmatrix} \dfrac{dw_I}{dr} \\ w_I \end{pmatrix}$ and $\begin{pmatrix} \dfrac{dw_{II}}{dr} \\ w_{II} \end{pmatrix}$ become equal at $r = L$:

$$\Omega_0^L(A_I) \begin{pmatrix} 1 \\ 0 \end{pmatrix} C_1 = e^{-\sqrt{k|\lambda|}\, L} \begin{pmatrix} -\sqrt{k|\lambda|} \\ 1 \end{pmatrix} C_2. \tag{2.13}$$

Since $C_1 \neq 0$ and $C_2 \neq 0$, we must have

$$\det\left\{ \Omega_0^L(A_I) \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \begin{matrix} -\sqrt{k|\lambda|} \\ 1 \end{matrix} \right\} = 0. \tag{2.14}$$

This is the equation which must be satisfied by the discrete eigenvalues of the eigenvalue problem (2.1). The problem of determining the discrete part of the spectrum of (2.1) is thus reduced to the problem of forming the matrizant $\Omega_0^L(A_I)$. In general, the left-hand side of (2.14) will appear as an absolutely convergent power series in $\sqrt{k|\lambda|}$.

The eigenfunction of (2.1), which belongs to the eigenvalue obtained from (2.14), will be, according to (2.2), (2.7) and (2.8a),

$$R(r) = \begin{cases} \dfrac{1}{r}\left\{(0,\ 1)\,\Omega_0^r(A_I)\begin{pmatrix}1\\0\end{pmatrix}\right\}_{\lambda=\lambda_i} C_1 \ \text{ for } r\,\varepsilon\,[0,\ L] \\[2ex] \dfrac{1}{r}\,e^{\sqrt{k|\lambda_i|}\,r}\,\varkappa\,|\lambda_i|\,C_1 \ \text{ for } r\,\varepsilon\,[L,\infty]. \end{cases} \tag{2.15}$$

The factor $\varkappa(|\lambda_i|)$ is obtained from (2.13) and the constant C_1 determined from a normalizing condition. As is seen from (3.1c) below, $R(r)$ behaves at the origin as was required in (2.1).

3. Procedures for Forming the Matrizant $\Omega_0^r(A_I)$

Because of the special form of A_I the matrizant $\Omega_0^r(A_I)$ may be formed rather easily [(2)] [(3)]:

$$\left.\begin{aligned} \{\Omega_0^r(A_I)\}_{11} &= 1 - k\int_0^r(|\lambda| + V(r_1))\,dr_1\int_0^{r_1}dr_2 \\ &+ k^2\int_0^r(|\lambda|+V(r_1))\,dr_1\int_0^{r_1}dr_2\int_0^{r_2}(|\lambda|+V(r_3))\,dr_3\int_0^{r_3}dr_4 + \dots \end{aligned}\right\} \tag{3.1 a}$$

$$\left.\begin{aligned} \{\Omega_0^r(A_I)\}_{12} &= -k\int_0^r(|\lambda|+V(r_1))\,dr_1 \\ &+ k^2\int_0^r(|\lambda|+V(r_1))\,dr_1\int_0^{r_1}dr_2\int_0^{r_2}(|\lambda|+V(r_3))\,dr_3 + \dots . \end{aligned}\right\} \tag{3.1 b}$$

$$\{\Omega_0^r(A_I)\}_{21} = r - k\int_0^r dr_1\int_0^{r_1}(|\lambda|+V(r_2))\,dr_2\int_0^{r_2}dr_3 + \dots . \tag{3.1 c}$$

$$\left.\begin{aligned} \{\Omega_0^r(A_I)\}_{22} &= 1 - k\int_0^r dr_1\int_0^{r_1}(|\lambda|+V(r_2))\,dr_2 \\ &+ k^2\int_0^r dr_1\int_0^{r_1}(|\lambda|+V(r_2))\,dr_2\int_0^{r_2}dr_3\int_0^{r_3}(|\lambda|+V(r_4))\,dr_4 + \dots . \end{aligned}\right\} \tag{3.1 d}$$

It remains, however, to rearrange these into a power series in $|\lambda|$.

In the following we shall introduce a procedure which yields more directly the matrizant as a power series in λ. First, however, we write the potential function $V(r)$ into the more convenient form

$$V(r) = -V_0 + V_0 w\left(\frac{r}{L}\right),$$

where $-V_0 = \min V(r)$ and where $w(\xi)$ is a function integrable in the Lebesgue sense over the interval $[0, 1]$ such that $w\left(\frac{r}{L}\right) = 1$ for $r \varepsilon (L, \infty]$. Then we rewrite the matrix A_I as follows:

$$\left.\begin{aligned} A_I &= \begin{pmatrix} 0 & k\left(|\lambda| - V_0 + V_0 w\left(\frac{r}{L}\right)\right) \\ 1 & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & \frac{1}{L^2}\lambda_0^2 w\left(\frac{r}{L}\right) \\ 1 & 0 \end{pmatrix} + \frac{1}{L^2}(\lambda^2 - \lambda_0^2)\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \\ &= A_{I_0} + \frac{1}{L^2}(\lambda^2 - \lambda_0^2)\, A_I, \end{aligned}\right\} \tag{3.2}$$

where we introduce the dimensionless quantities $\lambda^2 = k|\lambda|L^2$ and $\lambda_0^2 = kV_0L^2$. By applying the property 3° of the matrizant we obtain

$$\Omega_0^r(A_I) = \Omega_0^r(A_{I_0})\, \Omega_0^r\left\{[\Omega_0^r(A_{I_0})]^{-1} A_{I_1} \Omega_0^r(A_{I_0}) \frac{\lambda^2 - \lambda_0^2}{L^2}\right\}. \tag{3.3}$$

The second term on the right-hand side now appears as a power series in $|\lambda|$. The convergence of this series for all $r \varepsilon [0, L]$ and, as a matter of fact, the existence of such a power series, follow directly from the properties of the matrizant.

We see that the forming of the matrizant $\Omega_0^r(A_I)$ will take place by the following four steps:

1° The forming of $\Omega_0^r(A_{I_0})$.
2° The forming of $[\Omega_0^r(A_{I_0})]^{-1}$.
3° The forming of the matrix $S = [\Omega_0^r(A_{I_0})]^{-1} A_{I_0} \Omega_0^r(A_{I_0})$.
4° The forming of the matrizant $\Omega_0^r\left(\frac{\lambda^2 - \lambda_0^2}{L^2} S\right)$.

Step 1°: The matrizant $\Omega_0^r(A_{I_0})$ is formed most conveniently by means of the following relationship [4]:

$$\Omega_0^r\begin{pmatrix} 0 & \frac{1}{L^2}\lambda_0^2 w\left(\frac{r}{L}\right) \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} \Omega_{11}(\xi) & \frac{1}{L}\lambda_0^2 \int_0^\xi w(\xi_1)\,\Omega_{22}(\xi_1)\,d\xi_1 \\ L\int_0^\xi \Omega_{11}(\xi_1)\,d\xi_1 & \Omega_{22}(\xi) \end{pmatrix} \tag{3.4}$$

with

$$\left.\begin{aligned} \xi &= \frac{r}{L} \\ \Omega_{11}(r) &= \sum_{n=0}^{\infty} \lambda_0^{2n}\, a_{2n}^{(1)}(\xi) \\ \Omega_{22}(r) &= \sum_{n=0}^{\infty} \lambda_0^{2n}\, a_{2n}^{(2)}(\xi) \\ a_{2n}^{(1)} &= \int_0^\xi w(\xi_1)\,d\xi_1 \int_0^{\xi_1} d\xi_2 \int_0^{\xi_2} w(\xi_3)\,d\xi_3 \ldots \int_0^{\xi_{2n-2}} w(\xi_{2n-1})\,d\xi_{2n-1} \int_0^{\xi_{2n-1}} d\xi_{2n} \\ a_{2n}^{(2)} &= \int_0^\xi d\xi_1 \int_0^{\xi_1} w(\xi_2)\,d\xi_2 \int_0^{\xi_2} d\xi_3 \ldots \int_0^{\xi_{2n-2}} d\xi_{2n-1} \int_0^{\xi_{2n-1}} w(\xi_{2n})\,d\xi_{2n} \\ a_0^{(1)} &= 1 \\ a_0^{(2)} &= 1\,. \end{aligned}\right\} \tag{3.5}$$

Step 2°: The inversion of $\Omega_0^r(A_{I_0})$ is particularly easy to carry out:

$$[\Omega_0^r(A_{I_0})]^{-1} = \begin{pmatrix} \Omega_{11} & \Omega_{12} \\ \Omega_{21} & \Omega_{22} \end{pmatrix}^{-1} = [\det \Omega_0^r(A_{I_0})]^{-1} \begin{pmatrix} \Omega_{22} & -\Omega_{12} \\ -\Omega_{21} & \Omega_{11} \end{pmatrix}.$$

But according to the property 5° of the matrizant, since $Tr\, A_{I_0} = 0$, we have $\det \Omega_0^r(A_{I_0}) = 1$.
Hence

$$[\Omega_0^r(A_{I_0})]^{-1} = \begin{pmatrix} \Omega_{22} & -\Omega_{12} \\ -\Omega_{21} & \Omega_{11} \end{pmatrix}. \tag{3.6}$$

Step 3°: Both $\Omega_0^r(A_{I_0})$ and $[\Omega_0^r(A_{I_0})]^{-1}$ converge absolutely for all $r\,\varepsilon\,[0, L]$. Consequently we may form the product

$$[\Omega_0^r(A_{I_0})]^{-1} A_{I_1} \Omega_0^r(A_{I_0}),$$

which will also be an absolutely convergent series for all $r \varepsilon [0, L]$. By using (3.4), (3.5) and (3.6) we obtain

$$[\Omega_0^r(A_{I_0})]^{-1}\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}\Omega_0^r(A_{I_0}) = \sum_{q=0}^{\infty}\lambda_0^{2q}A_{2q} \tag{3.7}$$

with

$$A_{2q} = \sum_{m=0}^{q}\begin{pmatrix} La_{2m}^{(2)}(\xi)\left(\int_0^{\xi}a_{2(q-m)}^{(1)}(\xi_1)\,d\xi_1\right) & a_{2m}^{(2)}(\xi)\,a_{2(q-m)}^{(2)}(\xi) \\ -L^2\left(\int_0^{\xi}a_{2m}^{(1)}(\xi_1)\,d\xi_1\right)\left(\int_0^{\xi}a_{2(q-m)}^{(1)}(\xi_1)\,d\xi_1\right) & -L\left(\int_0^{\xi}a_{2m}^{(1)}(\xi_1)\,d\xi_1\right)a_{2(q-m)}^{(2)}(\xi). \end{pmatrix} \tag{3.8}$$

Step 4°: By using (3.7) we now obtain

$$\left.\begin{aligned}
&\Omega_0^r\left\{[\Omega_0^r(A_{I_0})]^{-1}\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}\Omega_0^r(A_{I_0})\frac{\lambda^2-\lambda_0^2}{L^2}\right\} \\
&= \sum_{n=0}^{\infty}(\lambda^2-\lambda_0^2)^n\left\{\sum_{i_n=0}^{\infty}\lambda_0^{2i_n}\left[\sum_{i_{n-1}=0}^{i_n}\sum_{i_{n-2}=0}^{i_{n-1}}\cdots\right.\right. \\
&\quad \cdots\sum_{i_2=0}^{i_3}\sum_{i_1=0}^{i_2}\int_0^{\frac{r}{L}}A_{2i_1}(\xi_1)\,d\xi_1\int_0^{\xi_1}A_{2(i_2-i_1)}(\xi_2)\,d\xi_2\cdots \\
&\quad \left.\left.\cdots\int_0^{\xi_{i_{n-2}}}A_{2(i_{n-1}-i_{n-2})}\left(\xi_{i_{n-1}}\right)d\xi_{i_{n-1}}\int_0^{\xi_{i_{n-1}}}A_{2(i_n-i_{n-1})}\left(\xi_{i_n}\right)d\xi_{i_n}\right]\right\} \\
&= I+(\lambda^2-\lambda_0^2)\left\{\sum_{i_1=0}^{\infty}\lambda_0^{2i_1}\int_0^{\frac{r}{L}}A_{2i_1}(\xi_1)\,d\xi_1\right\} \\
&\quad +(\lambda^2-\lambda_0^2)^2\left\{\sum_{i_2=0}^{\infty}\lambda_0^{2i_2}\left[\sum_{i_1=0}^{i_2}\int_0^{\frac{r}{L}}A_{2i_1}(\xi_1)\,d\xi_1\int_0^{\xi_1}A_{2(i_2-i_1)}(\xi_2)\,d\xi_2\right]\right\} \\
&\quad +(\lambda^2-\lambda_0^2)^3\left\{\sum_{i_3=0}^{\infty}\lambda_0^{2i_3}\right. \\
&\quad \left.\times\left[\sum_{i_2=0}^{i_3}\sum_{i_1=0}^{i_2}\int_0^{\frac{r}{L}}A_{2i_1}(\xi_1)\,d\xi_1\int_0^{\xi_1}A_{2(i_2-i_1)}(\xi_2)\,d\xi_2\int_0^{\xi_2}A_{2(i_3-i_2)}(\xi_3)\,d\xi_3\right]\right\} \\
&\quad +\cdots.
\end{aligned}\right\} \tag{3.9}$$

The absolute convergence of the above series follows from the absolute convergence of the matrizant and of the series (3.7).

In practical applications one would use, instead of (3.9), an approximate expression consisting of a finite number of terms. The accuracy of the approximation is easy to control when the formula (3.9) is applied.

We shall now consider the simplest eigenvalue problem of *CASE I*, i. e. the square well, applying to it the formulae (3.4) and (3.9)[1].

It is clear from these formulae that the treatment of a more general case would be essentially the same.

Now we have

$$\begin{aligned} A_I &= A_{I_0} + \frac{1}{L^2}(\lambda^2 - \lambda_0^2)\, A_{I_1} \\ &= \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \frac{1}{L^2}(\lambda^2 - \lambda_0^2)\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \end{aligned}$$

from which it follows that

$$\Omega_0^r (A_{I_0}) = \begin{pmatrix} 1 & 0 \\ L\xi & 1 \end{pmatrix} \tag{3.11}$$

and

$$[\Omega_0^r (A_{I_0})]^{-1} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \Omega_0^r (A_{I_0}) = \begin{pmatrix} L\xi & 1 \\ -L^2\xi^2 & -L\xi \end{pmatrix}.$$

Hence

$$A_0 = \begin{pmatrix} L\xi & 1 \\ -L^2\xi^2 & -L\xi \end{pmatrix}, \text{ but } A_{2q} = 0, \text{ as } q > 0.$$

We then obtain from (2.14), (3.9) and (3.11)

[1] Actually the matrizant method yields the well-known transcendental equation

$$\cot \sqrt{\lambda_0^2 - \lambda^2} = \sqrt{\frac{\lambda^2}{\lambda_0^2 - \lambda^2}} \tag{3.10}$$

for the discrete eigenvalues in the case of a square well. If we make use of the fact that A_I is now a constant matrix, we first obtain (3)

$$\Omega_0^r (A_I) = \exp(A_I r) = \begin{pmatrix} \cos\sqrt{\lambda_0^2 - \lambda^2}\,\xi & \frac{1}{L}\sqrt{\lambda_0^2 - \lambda^2}\,\sin\sqrt{\lambda_0^2 - \lambda^2}\,\xi \\ \frac{L}{\sqrt{\lambda_0^2 - \lambda^2}}\,\sin\sqrt{\lambda_0^2 - \lambda^2}\,\xi & \cos\sqrt{\lambda_0^2 - \lambda^2}\,\xi \end{pmatrix},$$

after which the above formula is easily derived from (2.14).

$$\lambda = \frac{1-\frac{1}{2}(\lambda_0^2-\lambda^2)+\frac{1}{24}(\lambda_0^2-\lambda^2)^2-\frac{1}{720}(\lambda_0^2-\lambda^2)^3+\dots}{1-\frac{1}{6}(\lambda_0^2-\lambda^2)+\frac{1}{120}(\lambda_0^2-\lambda^2)^2-\frac{1}{5040}(\lambda_0^2-\lambda^2)^3+\dots}.$$

Let us choose $\lambda_0^2 = 4$, in which case there will be only one discrete eigenvalue. Our formula gives $\lambda^2 = 0.4102$, and the exact formula (3.10) gives $\lambda^2 = 0.407118$. The error thus amounts only to about 0.74 per cent.

4. *Case II*

We now have $l \neq 0$, $a \neq 0$, and $b \neq 0$ in (1.1) and (1.2):

$$\left.\begin{aligned} &\frac{d^2R}{dr^2}+\frac{2}{r}\frac{dR}{dr}-\left[k|\lambda|+\frac{l(l+1)+ka}{r^2}-\frac{kb}{r}-kV_0\right]R = 0 \\ &R(0)<\infty \text{ and } R(r)\to 0, \text{ as } r\to\infty, \end{aligned}\right\} \tag{4.1}$$

where $|\lambda|$ is again the absolute value of the negative discrete eigenvalue. It is convenient to replace r by the dimensionless parameter $s=\frac{r}{\sigma}$, σ being a length suitable for the problem considered:

$$\left.\begin{aligned} &\frac{d^2R}{ds^2}+\frac{2}{s}\frac{dR}{ds}-\left(\Lambda+\frac{l(l+1)+A}{s^2}-\frac{G}{s}-V_1(s)\right)R = 0 \\ &R(0)<\infty \text{ and } R(s)\to 0, \text{ as } s\to\infty, \end{aligned}\right\} \tag{4.2}$$

where we have written

$$\Lambda = k\sigma^2|\lambda|,\ A = ka,\ G = k\sigma b, \text{ and } V_1(s) = k\sigma^2 V_0(\sigma s).$$

We must again find the solution of (4.2) separately for $s\varepsilon\left[0, \frac{L}{\sigma}\right]$, where $V_1(s) \neq 0$, and for $s\varepsilon\left[\frac{L}{\sigma}, \infty\right]$, where $V_1(s) \equiv 0$. The equation for the eigenvalues is then obtained, as in section 2, from the condition that these solutions must be equal for $s=\frac{L}{\sigma}$.

We substitute

$$R = s^p w(s), \tag{4.3}$$

where $p=\sqrt{\left(l+\frac{1}{2}\right)^2+A}-\frac{1}{2}$, in (4.2) and find by a straightforward calculation

$$\left.\begin{aligned}&\frac{d}{ds}\begin{pmatrix}\dfrac{dw}{ds}\\ w\end{pmatrix}-\left\{\frac{1}{s}\begin{pmatrix}-2(p+1) & -G\\ 0 & 0\end{pmatrix}+\begin{pmatrix}0 & \Lambda-V_1(s)\\ 1 & 0\end{pmatrix}\right\}\begin{pmatrix}\dfrac{dw}{ds}\\ w\end{pmatrix}=0\\ &\begin{pmatrix}\dfrac{dw}{ds}\\ w\end{pmatrix}_{s=0}<\infty \text{ and } \begin{pmatrix}\dfrac{d}{ds}(s^p w)\\ s^p w\end{pmatrix}\to 0,\ \text{as } s\to\infty.\end{aligned}\right\} \tag{4.4}$$

The matrix differential equation (4.4) is of the form

$$\frac{dz}{ds}-\left(\frac{P_{-1}}{s}+P\right)z=0 \tag{4.5}$$

with

$$z=\begin{pmatrix}\dfrac{dw}{ds}\\ w\end{pmatrix},\quad P_{-1}=\begin{pmatrix}-2(p+1) & -G\\ 0 & 0\end{pmatrix}\quad\text{and } P=\begin{pmatrix}0 & \Lambda-V_1(s)\\ 1 & 0\end{pmatrix}.$$

The solution of (4.5) is not the matrizant $\Omega_0^s\left(\frac{P_{-1}}{s}+P\right)$, because the elements of the matrix $\frac{P_{-1}}{s}+P$ are not all integrable over $\left[0, \frac{L}{\sigma}\right]$. We shall use temporarily the expression

$$\begin{pmatrix}\dfrac{dR}{ds}\\ R\end{pmatrix}=\Phi(s)\begin{pmatrix}0\\ 1\end{pmatrix}C_1 \tag{4.6}$$

for $s\,\varepsilon\left[0, \frac{L}{\sigma}\right]$ and postpone the determination of this form to the next section (the matrix $\Phi(s)$ is given there by (5.17)).

We now want to find a solution of (4.4) for $s\,\varepsilon\left(\frac{L}{\sigma}, \infty\right)$ (where $V_1(s)\equiv 0$) such that

$$\begin{pmatrix}\dfrac{dR}{ds}\\ R\end{pmatrix}\to\begin{pmatrix}0\\ 0\end{pmatrix},\quad\text{as } s\to\infty.$$

It will be convenient to start from the equation (4.2). By substituting

$$R(s)=\frac{w(x)}{x},\quad x=2\sqrt{\Lambda}\,s \tag{4.7}$$

we arrive at the Whittaker differential equation [7]

$$\frac{d^2 w}{dx^2} + \left(-\frac{1}{4} + \frac{k}{x} + \frac{\frac{1}{4} - m^2}{x^2} \right) w = 0, \tag{4.8}$$

where $k = \dfrac{G}{2\sqrt{\Lambda}}$ and $m = \sqrt{\left(l + \dfrac{1}{2}\right)^2 + A}$.

The general solution of (4.8) is, according to ref. (7),

$$w(x) = h_1 W_{k,m}(x) + h_2 W_{-k,m}(-x), \tag{4.9}$$

where

$$W_{k,m}(x) = \frac{e^{-\frac{x}{2}} x^k}{\Gamma\left(\frac{1}{2} - k + m\right)} \int_0^\infty t^{-k-\frac{1}{2}+m} \left(1 + \frac{t}{x}\right)^{k-\frac{1}{2}+m} e^{-t}\, dt \tag{4.10}$$

and where h_1 and h_2 are arbitrary constants. Since $W_{k,m}(x) \to 0$ but $W_{-k,m}(-x) \to \infty$, as $x \to \infty$, we must set $h_2 = 0$. The solution of (4.2) is thus given by

$$R(s) = \frac{h_1}{s} W_{k,m}\left(2\sqrt{\Lambda}\, s\right). \tag{4.11}$$

By making use of the identity (cf. ref. (7))

$$\frac{dW_{k,m}(x)}{dx} = \frac{k - \frac{1}{2}x}{x} W_{k,m}(x) - \frac{m^2 - \left(k - \frac{1}{2}\right)^2}{x} W_{k-1,m}(x) \tag{4.12}$$

we obtain

$$\left(\frac{\frac{dR}{ds}}{R}\right) = \frac{h_1}{s^2} \left(\frac{\left[k - \left(1 + \sqrt{\Lambda}\, s\right)\right] W_{k,m}\left(2\sqrt{\Lambda}\, s\right) - \left[m^2 - \left(k - \frac{1}{2}\right)^2\right] W_{k-1,m}\left(2\sqrt{\Lambda}\, s\right)}{s W_{k,m}\left(2\sqrt{\Lambda}\, s\right)} \right). \tag{4.13}$$

The solutions of (4.2) which are valid in the intervals $\left[0, \dfrac{L}{\sigma}\right]$ and $\left[\dfrac{L}{\sigma}, \infty\right]$ are given by (4.6) and (4.13) respectively. At the point $s = \dfrac{L}{\sigma}$ they must become equal:

$$\left.\begin{aligned}&\Phi\left(\frac{L}{\sigma}\right)\begin{pmatrix}0\\1\end{pmatrix}C_1\\&=\frac{h_1}{\left(\frac{L}{\sigma}\right)^2}\begin{pmatrix}\left[k-\left(1+\sqrt{A}\frac{L}{\sigma}\right)\right]W_{k,m}\left(2\sqrt{A}\frac{L}{\sigma}\right)-\left[m^2-\left(k-\frac{1}{2}\right)^2\right]W_{k-1,m}\left(2\sqrt{A}\frac{L}{\sigma}\right)\\\frac{L}{\sigma}W_{k,m}\left(2\sqrt{A}\frac{L}{\sigma}\right)\end{pmatrix}.\end{aligned}\right\}\quad(4.14)$$

In the same way as (2.14) was obtained from (2.13), we have from (4.14)

$$\det\left\{\Phi\left(\frac{L}{\sigma}\right)\begin{pmatrix}0\\1\end{pmatrix},\ \begin{matrix}\left[k-\left(1+\sqrt{A}\frac{L}{\sigma}\right)\right]W_{k,m}\left(2\sqrt{A}\frac{L}{\sigma}\right)-\left[m^2-\left(k-\frac{1}{2}\right)^2\right]W_{k-1,m}\left(2\sqrt{A}\frac{L}{\sigma}\right)\\\frac{L}{\sigma}W_{k,m}\left(2\sqrt{A}\frac{L}{\sigma}\right)\end{matrix}\right\}=0.\quad(4.15)$$

The equation (4.15) is now the equation for the discrete eigenvalues of (4.1). The solution of the eigenvalue problem (4.3) is thus reduced—if we consider the Whittaker function $W_{k,m}(x)$ as a standard function—to the forming of the matrix $\Phi\left(\frac{L}{\sigma}\right)$, a task which we shall undertake in the next section.

The eigenfunction $R_i(s)$ which corresponds to the eigenvalue A_i is obtained from (4.6), (4.11) and (4.15):

$$R_i(s)=\begin{cases}(0,\,1)\,[\Phi(s)]_{A=A_i}\begin{pmatrix}0\\1\end{pmatrix}C_1\ \text{for}\ s\,\varepsilon\left[0,\ \frac{L}{\sigma}\right]\\\frac{1}{s}W_{k,m}\left(2\sqrt{A_i}\,s\right)\varkappa(A_i)\,C_1\ \text{for}\ s\,\varepsilon\left[\frac{L}{\sigma},\ \infty\right],\end{cases}\quad(4.16)$$

where the factor $\varkappa(A_i)$ is defined by (4.14). The constant is obtained from a normalizing condition.

5. The Solution of the Matrix Differential Equation $\frac{dX}{ds}-\left(\frac{P_{-1}}{s}+P\right)X=0$

An excellent account of the properties of matrix differential equations of the form

$$\frac{dX}{ds}-\left(\frac{P_{-1}}{s}+P(s)\right)X=0$$

may be found in the book by GANTMACHER [(1)].

The following theorem, a special case of a more general theorem by GAMTMACHER (1), holds true:

Theorem: If (1°) the power series of

$$P(s) = \frac{P_{-1}}{s} + \sum_{m=0}^{\infty} P_m s^m$$

is convergent for $s \varepsilon \left[0, \frac{L}{\sigma}\right]$, and if (2°) no two eigenvalues of P_{-1} differ by an integer, then the solution of the matrix differential equation

$$\frac{dX}{ds} - P(s) X = 0 \tag{5.1}$$

will be of the form

$$X = A(s) \exp(P_{-1} \ln s) = A(s) s^{P_{-1}}, \tag{5.2}$$

where the matrix function $A(s)$ is regular at $s = 0$ and where $A(0) = I$.

Our matrix differential equation (4.5) satisfied the conditions 1° and 2° of the theorem. Indeed, according to what was said on page 3, the matrix $P(s)$ may be expressed as a power series

$$P(s) = \sum_{m=0}^{\infty} P_m s^m$$

absolutely convergent for $s \varepsilon \left[0, \frac{L}{\sigma}\right]$. Furthermore, the eigenvalues of P_{-1} are zero and $-2(p+1) = -\left[\sqrt{(2l+1)^2 + 4ak} + 1\right]$, where, according to our assumption about l and a, the eigenvalue $-2(p+1)$ is not an integer.

Our problem is now to form $A(s)$. This we could do (cf. refs. (1) and (6)) by forming and solving an infinite set of equations for the matrices A_n of

$$A(s) = \sum_{n=0}^{\infty} A_n s^n.$$

But this would be nothing else than solving (4.1) by the power series substitution

$$R(s) = s^p \sum_{n=0}^{\infty} a_n s^n,$$

a procedure which would not be very efficient. In the following we shall develop a procedure which is very similar to that employed in section 3.

It will be convenient to replace the matrix X of (5.1) by the new unknown matrix Y defined as follows [1]:

$$Y = TXT^{-1}, \tag{5.3}$$

where

$$T = \begin{pmatrix} 1 & \dfrac{G}{2(p+1)} \\ 0 & 1 \end{pmatrix}.$$

We then obtain from (4.4) the following differential equation for Y:

$$\frac{dY}{ds} - \left(\frac{\theta}{s} + \gamma(s)\right) Y = 0, \tag{5.4}$$

where

$$\theta = \begin{pmatrix} -2(p+1) & 0 \\ 0 & 0 \end{pmatrix} \tag{5.4 a}$$

and

$$\gamma(s) = \begin{pmatrix} \beta & -\beta^2 + A - V_1(s) \\ 1 & -\beta \end{pmatrix}, \quad \beta = \frac{G}{2(p+1)}.$$

According to the theorem on page 18 the solution of (5.4) will be of the form

$$Y = A(s)\, s^{\theta}, \tag{5.5}$$

where $A(s)$ is regular in $\left[0, \dfrac{L}{\sigma}\right]$. The substitution of (5.5) in (5.4) yields the following equation for $A(s)$:

$$\frac{dA}{ds} + \frac{1}{s}(A\theta - \theta A) - \gamma A = 0. \tag{5.6}$$

We substitute here, as Erougin does in a different connection [5],

$$A = s^{\theta}\, C(s)\, s^{-\theta} \tag{5.7}$$

and obtain the following differential equation for $C(s)$:

$$\frac{dC}{ds} - B(s)\, C = 0, \tag{5.8}$$

where

$$\left.\begin{aligned} B(s) &= s^{-\theta}\,\gamma s^{\theta} = \begin{pmatrix} \beta & [-\beta^2 + \Lambda - V_1(s)]\,s^{\alpha} \\ s^{-\alpha} & -\beta \end{pmatrix}, \\ \alpha &= 2\,(p+1) \text{ and } \beta = \frac{G}{\alpha}. \end{aligned}\right\} \tag{5.9}$$

The equation (5.8) is satisfied for $s\,\varepsilon \left(s_0, \frac{L}{\sigma}\right]$, $s_0 > 0$, by the matrix series

$$\tilde{\Omega}\,(B) = I + \int^{s} B\,ds_1 + \int^{s} B\,ds_1 \int^{s_1} B\,ds_2 + \ldots, \tag{5.10}$$

where, in carrying out the integrations, we put constants of integration equal to zero in all terms. The uniform and absolute convergence of (5.10) for $s\,\varepsilon \left(s_0, \frac{L}{\sigma}\right]$, $s_0 > 0$, is easy to verify. Consequently

$$A\,(s) = I + s^{\theta}\left(\int^{s} B\,ds_1\right)s^{-\theta} + s^{\theta}\left(\int^{s} B\,ds_1 \int^{s_1} B\,ds_2\right)s^{-\theta} + \ldots. \tag{5.11}$$

is an absolutely and uniformly convergent series for $s\,\varepsilon \left(s_0, \frac{L}{\sigma}\right]$. But the series (5.11) converges in an arbitrary neighbourhood of the origin.

Indeed, if

$$\eta_0 = \max\left\{\beta,\ 1 - \beta^2 + \Lambda - V_1(s),\ -\beta,\ 1\right\},$$

we have

$$\int^{s} B\,ds_1 \leqslant \eta_0\, s \begin{pmatrix} 1 & s^{\alpha} \\ s^{-\alpha} & 1 \end{pmatrix}$$

$$\int^{s} B\,ds_1 \int^{s_1} B\,ds_2 \leqslant 2\,\eta_0^2\, s^2 \begin{pmatrix} 1 & s^{\alpha} \\ s^{-\alpha} & 1 \end{pmatrix}$$

$$\vdots$$

$$\int^{s} B\,ds_1 \int^{s_1} \ldots \int^{s_n} B\,ds_{n+1} \leqslant 2^{n-1}\,\eta_0^n\, s^n \begin{pmatrix} 1 & s^{\alpha} \\ s^{-\alpha} & 1 \end{pmatrix},$$

as is easily shown by induction. Here use has been made also of the fact that $\alpha \geqslant 2$. Hence

$$s^{\theta}\int^{s} B\,ds_1 \int^{s_1} B\,ds_2 \ldots \int^{s_n} B\,ds_{n+1}\, s^{-\theta} \leqslant 2^{n-1}\,\eta_0^n\, s^n \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

The series (5.11) thus converges absolutely and uniformly for $s \varepsilon \left[0, \frac{1}{2\eta_0}\right)$, $0 < \eta_0 < \infty$. It follows that the matrix series $s^\theta \tilde{\Omega}(B) s^{-\theta}$ converges absolutely and uniformly and satisfies the differential equation (5.4) in the whole interval $\left[0, \frac{L}{\sigma}\right]$. Since $V_1(s)$ in (5.9) is an absolutely convergent power series in s, it follows—as would be easy to show—that all terms of (5.11) have power series in s as elements. Besides, $s^\theta \tilde{\Omega}(B) s^{-\theta} \to I$, as $s \to 0$. From the theorem on page 18 we conclude that

$$Y = \left\{ s^\theta \tilde{\Omega}(B) s^{-\theta} \right\} s^\theta \tag{5.12}$$

is a solution of (5.4) (we do not write $Y = s^\theta \tilde{\Omega}(B)$ since we want our solution to appear in the form suggested by the theorem). From (5.3) it follows that the general solution of (4.5) is given by

$$z = T^{-1} \left\{ s^\theta \tilde{\Omega}(B) s^{-\theta} \right\} s^\theta T z_0, \tag{5.13}$$

where z_0 is an arbitrary vector. From (4.3) and (5.13) it is then seen that

$$\begin{pmatrix} \frac{dR}{ds} \\ R \end{pmatrix} = s^{p-1} \begin{pmatrix} s & p \\ o & s \end{pmatrix} T^{-1} \left\{ s^\theta \tilde{\Omega}(B) s^{-\theta} \right\} s^\theta T z_0. \tag{5.14}$$

The vector z_0 must be chosen so that the condition $R(0) < \infty$ (cf. (4.2)) is fulfilled. Now

$$s^\theta T z_0 = \begin{pmatrix} s^{-2(p+1)} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & \frac{G}{2(p+1)} \\ 0 & 1 \end{pmatrix} z_0 = \begin{pmatrix} s^{-2(p+1)} & s^{-2(p+1)} \frac{G}{2(p+1)} \\ 0 & 1 \end{pmatrix} z_0. \tag{5.15}$$

From (5.14) and (5.15) it is clear that we must set

$$z_0 = \begin{pmatrix} -\frac{G}{2(p+1)} \\ 1 \end{pmatrix} C_1,$$

C_1 being a constant. Finally we obtain

$$\begin{pmatrix} \frac{dR}{ds} \\ R \end{pmatrix} = s^{p-1} \begin{pmatrix} s & p - \frac{G}{2(p+1)} s \\ 0 & s \end{pmatrix} \left\{ s^\theta \tilde{\Omega}(B) s^{-\theta} \right\} \begin{pmatrix} 0 \\ 1 \end{pmatrix} C_1. \tag{5.16}$$

The $\Phi(s)$-matrix of (4.6), (4.14), (4.15), and (4.16) is thus

$$\Phi(s) = s^{p-1} \begin{pmatrix} s & p - \dfrac{G}{2\,(p+1)}\, s \\ 0 & s \end{pmatrix} \left\{ s^{\theta}\, \tilde{\Omega}\, (s^{-\theta}\, \gamma\, s^{\theta})\, s^{-\theta} \right\}, \tag{5.17}$$

the matrix γ having been defined in (5.4a).

The eigenvalue Λ is contained in γ. In practical applications one prefers, however, to have the matrix $\Phi(s)$ in the form of a power series in Λ. In order to achieve this, we first rewrite γ as follows:

$$\gamma = \gamma_1 + \Lambda\, \gamma_2,$$

where

$$\gamma_1 = \begin{pmatrix} \beta & -\beta^2 - V_1(s) \\ 1 & -\beta \end{pmatrix} \text{ and } \gamma_2 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

The differential equation (5.6) will then appear in the form

$$\frac{dA}{ds} + \frac{1}{s}(A\,\theta - \theta\, A) - (\gamma_1 + \Lambda\, \gamma_2)\, A = 0. \tag{5.18}$$

We substitute

$$A = A_1\, D, \tag{5.19}$$

with

$$A_1 = s^{\theta}\, \tilde{\Omega}\, (s^{-\theta}\, \gamma_1\, s^{\theta})\, s^{-\theta},$$

in (5.18). As is seen at once, A_1 is the solution of

$$\left.\begin{aligned} &\frac{dA_1}{ds} + \frac{1}{s}(A_1\theta - \theta A_1) \; - \gamma_1\, A_1 = 0 \\ &A_1(0) = I. \end{aligned}\right\} \tag{5.20}$$

Remembering that the inverse of A_1 exists for every $s \varepsilon \left[0, \dfrac{L}{\sigma}\right]$ (cf. ref. (6)), we obtain the differential equation

$$\frac{dD}{ds} + \frac{1}{s}(D\theta - \theta D) - \Lambda\, (A_1^{-1}\, \gamma_2\, A_1)\, D = 0 \tag{5.21}$$

for D. Since $A(0) = A_1(0) = I$, we require that $D(0) = I$. Before we are able to write down the solution of (5.21), we have to consider the matrix $A_1^{-1}\gamma_1 A_1$ a little more closely. Instead of directly inverting the matrix A_1, we may proceed as follows: It is easy to verify that A_1^{-1} satisfies the differential equation

$$\frac{dY}{ds} + \frac{1}{s}\,(Y\theta - \theta Y) + Y\gamma_1 = 0 \tag{5.22}$$

and furthermore, when we require $Y(0) = I$, that

$$Y = s^{\theta}\,\tilde{\psi}\,(-s^{-\theta}\,\gamma_1\,s^{\theta})\,s^{-\theta} \tag{5.23}$$

for $s\,\varepsilon\left[0, \frac{L}{\sigma}\right]$, where

$$\tilde{\psi}\,(-F) = I - \int^{s} F\,ds_1 + \int^{s} ds_1 \left(\int^{s_1} F\,ds_2\right) F\,(s_1) - \dots . \tag{5.24}$$

(F standing for $s^{-\theta}\gamma_1 s^{\theta}$). The matrix $s^{\theta}\,\tilde{\psi}(s^{-\theta}\gamma_1 s^{\theta})\,s^{-\theta}$ is an absolutely and uniformly convergent power series in s, as is easy to show by a procedure practically identical with the one used in connection with (5.11). It follows that the matrix $\Lambda\,A_1^{-1}\gamma_2 A_1$ is an absolutely and uniformly convergent power series in s. We conclude from this that the solution of (5.21) satisfying the condition $D(0) = I$ is given by the matrix

$$D = s^{\theta}\,\tilde{\Omega}\left\{\Lambda\,s^{-\theta}\,[s^{\theta}\,\tilde{\psi}\,(-s^{-\theta}\,\gamma_1\,s^{\theta})\,s^{-\theta}]\,\gamma_2\,[s^{\theta}\,\tilde{\Omega}\,(s^{-\theta}\,\gamma_1\,s^{\theta})\,s^{-\theta}]\,s^{\theta}\right\}s^{-\theta}. \tag{5.25}$$

Finally we obtain from (5.17), (5.19) and (5.25)

$$\left.\begin{aligned} \Phi(s) = s^{p-1} & \begin{pmatrix} s & p - \dfrac{G}{2\,(p+1)}\,s \\ 0 & s \end{pmatrix} s^{\theta}\,\tilde{\Omega}\,(s^{-\theta}\,\gamma_1\,s^{\theta})\,s^{-\theta} \\ s^{\theta}\,\tilde{\Omega}\{\Lambda\,s^{-\theta}\,[s^{\theta}\,\tilde{\psi}\,(-s^{-\theta}\,\gamma_1\,s^{\theta})\,s^{-\theta}]\,\gamma_2\,&[s^{\theta}\,\tilde{\Omega}\,(s^{-\theta}\,\gamma_1\,s^{\theta})\,s^{-\theta}]\,s^{\theta}\}\,s^{-\theta}, \end{aligned}\right\} \tag{5.26}$$

which is clearly a power series in Λ. In (5.25) and (5.26) we have maintained the forms $s^{\theta}\,\Omega\,s^{-\theta}$ and $s^{\theta}\,\tilde{\psi}\,s^{-\theta}$ since they are matrices with power series in s as elements. Everything that was said in section 3 in connection with (3.3) will hold for (5.26).

Acknowledgements

I want to express my deep gratitude to Professor NIELS BOHR for excellent working conditions at the Institute for Theoretical Physics in Copenhagen.

Further I want to thank Professor L. ROSENFELD and Professor C. MØLLER for their suggestion to add an example to section 3, which led to a revision of the whole section.

I am greatly indebted to NORDITA for the research fellowship granted me by that institute.

NORDITA – Nordisk Institut for Teoretisk Atomfysik
Copenhagen, Denmark

References

(1) Ф. Р. Гантмахер, Теория Матриц (Гостехиздат, Москва, 1953).

(2) O. HELLMAN, Die Anwendung des Matrizanten bei Eigenwertaufgaben. Z. angew. Math. Mech. **35** (1955).

(3) O. HELLMAN, On the Solution of the One Dimensional Schrödinger Equation in Case of a Potential Well. Ann. Acad. Sci. Fennicae, Physica **6**, no. 11 (1958).

(4) O. HELLMAN, Ein Verfahren zur Bildung von Matrizanten. Z. angew. Math. Mech. **37** (1957).

(5) Н. П. Еругин, Приводимые системы. Труды математического инст. Стеклова XIII.

(6) E. A. CODDINGTON and N. LEVINSON, Theory of Ordinary Differential Equations (McGraw-Hill, New York, 1955).

(7) E. T. WHITTAKER, An Expression of Certain Known Functions as Generalized Hypergeometric Functions. Bull. Am. Math. Soc. **10** (1904) 125.

Indleveret til selskabet den 12. august 1959.
Færdig fra trykkeriet den 12. februar 1960.