Improvement on the WKB method using an algebraic formalism

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# Improvement on the WKB method using an algebraic formalism 

E G Sauter<br>Institut für Hochfrequenztechnik und Quantenelektronik, Universität Karlsruhe, 75 Karlsruhe 1, West Germany

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#### Abstract

The equation $\ddot{u}+w^{2}(t) u=0$ can be transformed to a system of two first-order differential equations $\dot{y}=M y$ by different ways of parametrisation. The method of decoupled exponents of Wei and Norman yields a Riccati differential equation for the unknown exponents and an easily interpretable solution $y$. A solution with vanishing exponents in the parametrisation of Mulholland corresponds exactly to the WKB method. Therefore an approximate solution of the Riccati differential equation gives an improvement on the WKB.


## 1. Introduction

Most of the linear differential equations (DE) in physics are of second order. In this paper we shall study an important subset of them, those DE which can be reduced to normal form (for the exact conditions, cf Kamke 1942)

$$
\begin{equation*}
\ddot{u}+w^{2}(t) u=0, \tag{1}
\end{equation*}
$$

or, after introducing a new variable by $u=\exp \left(\int v \mathrm{~d} t\right)$, to the equivalent Riccati DE

$$
\begin{equation*}
\dot{v}+v^{2}+w^{2}(t)=0 . \tag{2}
\end{equation*}
$$

We assume in the following that $w(t)$ is continuous in an interval $I_{t}$ containing $t=0$; then there exists a global and unique solution for given initial values $u(0), \dot{u}(0)$. Unfortunately, only little is known beyond this statement. Only a few types of de (1) allow a complete solution; some types have a theory of their own, but, in general, it is impossible to represent the solution by a finite number of quadratures and elementary functions. Therefore one has to have recourse to approximate methods of solution, for example to the WKB method. The condition for the applicability of the WKB method is a coefficient $w^{2}$ of the form $w^{2}(t)=F^{2}(t) / \lambda^{2}$ with a large factor $1 / \lambda$. The solution of (1) is expressed as an exponential $u=\exp (i S(t) / \lambda)$, where $S(t)$ is expanded in a power series in $\lambda$. The lowest-order solution then reads $u(t)=\exp \left( \pm \mathrm{i} \int w \mathrm{~d} t\right)$. Instead of going into details, we refer to two standard references (Morse and Feshbach 1953, Fröman and Fröman 1965). In § 2 we transform equation (1) into a form suitable for the following investigations by introducing the equivalent matrix $D E$ for the integral matrix $Q$ (fundamental solution matrix) and by extracting two simple factors from $Q$.

Some years ago, Wei and Norman $(1963,1964)$ proposed a solution of equation (1) based on Lie algebraic methods. This method cannot, of course, solve equations otherwise unsolvable; the solution is reduced to the solution of a certain Riccati DE.

However, the solution appears in a very appealing form, and it allows an easy improvement on the WKB method. As far as we know, this method has not found many applications in the literature-frequency modulation (Mulholland 1970, Mulholland and Machiraju 1973), light propagation (Strezh 1976), quantum mechanics (Chang and Light 1969, Flamand 1966)-presumably because Lie algebra is not sufficiently well known to physicists and engineers. Therefore we present in § 3 the method of decoupled exponentials of Wei and Norman in a form which uses only simple $2 \times 2$ matrix manipulations, thus avoiding the Lie algebraic language. In the main part, $\S 4$, we discuss the connection with the WKB method. In § 5 we give an example for the improvement on the WKB method by a perturbative solution of the Wei-Norman equations. In the Appendix some results from elementary matrix algebra are listed.

In the following, all 'vectors' are $2 \times 1$ matrices, all 'matrices' are $2 \times 2$ matrices.

## 2. Preparation of the differential equation

### 2.1. The $D E$ for the integral matrix $Q(t)$

Equation (1) can be put in the form of two coupled first-order DE

$$
\begin{equation*}
\dot{y}=M(t) y, \tag{3}
\end{equation*}
$$

where the components of

$$
\begin{equation*}
y=\binom{y_{1}}{y_{2}} \tag{4}
\end{equation*}
$$

are some linear combinations of $u$ and $\dot{u}$, and the components of

$$
M=\left(\begin{array}{ll}
m_{1}(t) & m_{2}(t)  \tag{5}\\
m_{3}(t) & m_{4}(t)
\end{array}\right)
$$

depend on $w(t)$. Now the ansatz

$$
\begin{equation*}
y(t)=Q(t) y(0) \tag{6}
\end{equation*}
$$

where

$$
\begin{equation*}
y(0)=\binom{y_{10}}{y_{20}}=\rho_{0}\binom{\sin \beta}{\cos \beta}, \tag{7}
\end{equation*}
$$

transforms equation (3) to the matrix DE for the integral matrix $Q$ :

$$
\begin{equation*}
\dot{Q}(t)=M(t) Q(t), \tag{8}
\end{equation*}
$$

with the initial condition

$$
Q(0)=\left(\begin{array}{ll}
1 & 0  \tag{9}\\
0 & 1
\end{array}\right)=\sigma_{0} .
$$

### 2.2. Three different parametrisations for $y$

We choose as a first parametrisation

$$
\begin{equation*}
y \rightarrow y_{\mathrm{I}}=\binom{y_{1}}{y_{2}}_{\mathrm{I}}=\binom{\dot{u}}{u} . \tag{10}
\end{equation*}
$$

Then

$$
M \rightarrow M_{\mathrm{I}}=\left(\begin{array}{cc}
0 & -w^{2}  \tag{11}\\
1 & 0
\end{array}\right) .
$$

One can get a whole class of admissible parametrisations by applying a Lyapunov transformation (Pease 1965) to $y_{\mathrm{i}}$ :

$$
\begin{equation*}
y_{\mathrm{I}}=B_{i}(t) y_{i} \quad(i=\mathrm{II}, \mathrm{III}, \ldots) \tag{12}
\end{equation*}
$$

Here $B(t)$ is continuously differentiable, $B(t)$ and $\dot{B}(t)$ are bounded, and the magnitude of $\operatorname{det} B(t)$ has a lower bound, in the interval $I_{t}$. Substituting this $t$-dependent coordinate transformation (12) into equation (3) (with index I), we obtain

$$
\begin{equation*}
\dot{y}_{i}=M_{i}(t) y_{i}, \quad \text { with } M_{i}=B_{i}^{-1} M_{\mathrm{I}} B_{i}-B_{i}^{-1} \dot{B}_{i} \tag{13}
\end{equation*}
$$

A Lyapunov transformation transforms $Q$ as follows:

$$
\begin{equation*}
Q_{\mathrm{I}}(t)=B_{i}(t) Q_{i}(t) B_{i}^{-1}(0) \tag{14}
\end{equation*}
$$

$i=$ II: With

$$
B_{\mathrm{II}}=\left(\begin{array}{cc}
\mathrm{i} w & -\mathrm{i} w  \tag{15}\\
1 & 1
\end{array}\right)
$$

(Van Kampen 1967) we get

$$
\begin{equation*}
y_{\mathrm{II}}=\binom{y_{1}}{y_{2}}_{\mathrm{II}}=\frac{1}{2}\binom{u-\mathrm{i} \dot{u} / w}{u+\mathrm{i} \dot{u} / w} \tag{16}
\end{equation*}
$$

and

$$
M_{\mathrm{II}}=\mathrm{i} w\left(\begin{array}{rr}
1 & 0  \tag{17}\\
0 & -1
\end{array}\right)-\frac{\dot{w}}{2 w}\left(\begin{array}{rr}
1 & -1 \\
-1 & 1
\end{array}\right) .
$$

$i=$ III: With

$$
B_{\mathrm{III}}=\left(\begin{array}{cc}
w & 0  \tag{18}\\
0 & 1
\end{array}\right)
$$

(Mulholland 1970) we get

$$
\begin{equation*}
y_{\mathrm{II}}=\binom{y_{1}}{y_{2}}_{\mathrm{III}}=\binom{\dot{u} / w}{u} \tag{19}
\end{equation*}
$$

and

$$
M_{\mathrm{III}}=\left(\begin{array}{cc}
-\dot{w} / w & -w  \tag{20}\\
w & 0
\end{array}\right) .
$$

These three parametrisations will not be used before § 4 .

### 2.3. Extraction of the trace part

$M$ from equation (5) is decomposed into

$$
\begin{equation*}
M=M_{\mathrm{T}}+M_{\mathrm{R}} \tag{21}
\end{equation*}
$$

where

$$
\begin{equation*}
M_{\mathrm{T}}=\frac{1}{2}\left(m_{1}+m_{4}\right) \sigma_{0}=\frac{1}{2} \sigma_{0} \operatorname{Tr} M(t) \tag{22}
\end{equation*}
$$

and

$$
M_{\mathrm{R}}=\left(\begin{array}{cc}
\left(m_{1}-m_{4}\right) / 2 & m_{2}  \tag{23}\\
m_{3} & -\left(m_{1}-m_{4}\right) / 2
\end{array}\right), \quad \text { with } \operatorname{Tr} M_{\mathrm{R}}=0
$$

With the factor decomposition of the integral matrix

$$
\begin{equation*}
Q=Q_{\mathrm{R}} Q_{\mathrm{T}} \tag{24}
\end{equation*}
$$

we get from equation (8) the two matrix DE

$$
\begin{equation*}
\dot{Q}_{\mathrm{T}}=\left(Q_{\mathrm{R}}^{-1} M_{\mathrm{T}} Q_{\mathrm{R}}\right) Q_{\mathrm{T}}=M_{\mathrm{T}} Q_{\mathrm{T}}=\frac{1}{2} Q_{\mathrm{T}} \operatorname{Tr} M(t), \quad Q_{\mathrm{T}}(0)=\sigma_{0} \tag{25}
\end{equation*}
$$

and

$$
\begin{equation*}
\dot{Q}_{\mathrm{R}}=M_{\mathrm{R}} Q_{\mathrm{R}}, \quad Q_{\mathrm{R}}(0)=\sigma_{0} \tag{26}
\end{equation*}
$$

According to theorem 1 of the Appendix, equation (25) can immediately be solved:

$$
\begin{equation*}
Q_{\mathrm{T}}(t)=\exp \left(\int_{0}^{t} M_{\mathrm{T}}(s) \mathrm{d} s\right)=\sigma_{0} \exp \left(\frac{1}{2} \int_{0}^{t} \operatorname{Tr} M(s) \mathrm{d} s\right) \tag{27}
\end{equation*}
$$

a multiple of the unit matrix.

### 2.4. Extraction of the antisymmetric part

Next we decompose $M_{R}$, equation (23), into

$$
\begin{equation*}
M_{\mathrm{R}}=M_{\mathrm{A}}+M_{\mathrm{S}} \tag{28}
\end{equation*}
$$

where the antisymmetric and the symmetric part are respectively

$$
M_{\mathrm{A}}=\frac{1}{2}\left(M_{\mathrm{R}}-M_{\mathrm{R}}^{\mathrm{T}}\right)=\frac{1}{2}\left(m_{2}-m_{3}\right)\left(\begin{array}{rr}
0 & 1  \tag{29}\\
-1 & 0
\end{array}\right)=\frac{1}{2}\left(m_{2}-m_{3}\right) X_{1}
$$

(see Appendix) and

$$
\boldsymbol{M}_{\mathrm{S}}=\frac{1}{2}\left(\boldsymbol{M}_{\mathrm{R}}+\boldsymbol{M}_{\mathrm{R}}^{\mathrm{T}}\right)=\frac{1}{2}\left(\begin{array}{cc}
m_{1}-m_{4} & m_{2}+m_{3}  \tag{30}\\
m_{2}+m_{3} & -\left(m_{1}-m_{4}\right)
\end{array}\right) .
$$

With the factor decomposition

$$
\begin{equation*}
Q_{\mathrm{R}}=Q_{\mathrm{A}} Q_{\mathrm{S}} \tag{31}
\end{equation*}
$$

we obtain from equation (26) the two $D E$

$$
\begin{array}{ll}
\dot{Q}_{\mathrm{A}}=M_{\mathrm{A}} Q_{\mathrm{A}}, & Q_{\mathrm{A}}(0)=\sigma_{0} \\
\dot{Q}_{\mathrm{S}}=T Q_{\mathrm{S}}, & Q_{\mathrm{S}}(0)=\sigma_{0} \tag{33}
\end{array}
$$

with

$$
\begin{equation*}
T=Q_{\mathrm{A}}^{-1} M_{\mathrm{s}} Q_{\mathrm{A}} \tag{34}
\end{equation*}
$$

Equation (32) can again be solved according to theorem 1: with

$$
\begin{equation*}
f(t)=\frac{1}{2} \int_{0}^{t}\left(m_{2}(s)-m_{3}(s)\right) \mathrm{d} s \tag{35}
\end{equation*}
$$

we find

$$
\begin{equation*}
Q_{\mathrm{A}}(t)=\exp \left(f(t) X_{1}\right)=\sigma_{0} \cos f+X_{1} \sin f=\binom{\cos f \sin f}{-\sin f \cos f} \tag{36}
\end{equation*}
$$

a two-dimensional rotation matrix. Here equation (77) has been used. Thus from (34):

$$
\begin{gather*}
T=\frac{1}{2}\left(\begin{array}{ll}
\left(m_{1}-m_{4}\right) \cos 2 f-\left(m_{2}+m_{3}\right) \sin 2 f & \left(m_{1}-m_{4}\right) \sin 2 f+\left(m_{2}+m_{3}\right) \cos 2 f \\
\left(m_{1}-m_{4}\right) \sin 2 f+\left(m_{2}+m_{3}\right) \cos 2 f & -\left(m_{1}-m_{4}\right) \cos 2 f+\left(m_{2}+m_{3}\right) \sin 2 f
\end{array}\right) \\
=\left(\begin{array}{rr}
t_{1} & t_{2} \\
t_{2} & -t_{1}
\end{array}\right) . \tag{37}
\end{gather*}
$$

Note that both the extraction of the trace part and the extraction of the antisymmetric part are Lyapunov transformations (with $B_{i}=Q_{\mathrm{T}}, Q_{\mathrm{A}}$ respectively).

## 3. The method of decoupled exponentials

### 3.1. Derivation of the Riccati DE for the exponents

We use the fact that each $2 \times 2$ matrix with vanishing trace can be represented by a linear combination of the Pauli matrices $\sigma_{1}, \sigma_{2}, \sigma_{3}$, or by some linear combination $X_{1}, X_{2}, X_{3}$ of the basic matrices $\sigma_{i}$ (see Appendix). Especially we have chosen

$$
\begin{equation*}
X_{1}=\mathrm{i} \sigma_{2}, \quad X_{2}=\sigma_{3}, \quad X_{3}=\left(\sigma_{1}+\mathrm{i} \sigma_{2}\right) / 2=\sigma_{+} \tag{38}
\end{equation*}
$$

Now the remaining DE (33) with $T$ from equation (37) can be solved at least locally in the form

$$
\begin{equation*}
Q_{\mathrm{S}}(t)=\exp \left(\sum_{i} h_{i}(t) X_{i}\right), \tag{39}
\end{equation*}
$$

but in general not globally (Magnus 1954, Wichmann 1961). However, Wei and Norman $(1963,1964)$ and Wei $(1963)$ have shown that the ansatz

$$
\begin{equation*}
Q_{\mathrm{S}}(t)=\prod_{i=1}^{3} \exp \left(g_{i}(t) X_{i}\right), \quad \text { where } g_{i}(0)=0 \tag{40}
\end{equation*}
$$

of decoupled exponentials is superior to the form (39); in the case of a $2 \times 2$ matrix, this solution holds globally if a suitable basis $X_{i}$ is chosen. Besides (38) there are other combinations of the matrices $\sigma_{1}, \sigma_{2}, \sigma_{3}$ which will do it too (but not the original Pauli matrices, for example). One could have applied a corresponding factorisation immediately to the DE (8); however, we have preferred first to simplify the DE as far as possible. Explicitly, we have (cf equations (75), (76), (77))

$$
\begin{align*}
Q_{\mathrm{s}}(t)=\mathrm{e}^{g_{1} X_{1}} & \mathrm{e}^{g_{2} x_{2}} \mathrm{e}^{g_{3} X_{3}} \\
& =\left(\begin{array}{cc}
\cos g_{1} & \sin g_{1} \\
-\sin g_{1} & \cos g_{1}
\end{array}\right)\left(\begin{array}{cc}
\exp g_{2} & 0 \\
0 & \exp \left(-g_{2}\right)
\end{array}\right)\left(\begin{array}{cc}
1 & g_{3} \\
0 & 1
\end{array}\right) \\
& =\left(\begin{array}{cc}
\cos g_{1} \exp g_{2} & g_{3} \cos g_{1} \exp g_{2}+\sin g_{1} \exp \left(-g_{2}\right) \\
-\sin g_{1} \exp g_{2} & -g_{3} \sin g_{1} \exp g_{2}+\cos g_{1} \exp \left(-g_{2}\right)
\end{array}\right) . \tag{41}
\end{align*}
$$

Substitution into equation (33) yields a system of four equations, which we want to solve for the three derivatives $\dot{g}_{i}$. This system is consistent; the solution is

$$
\begin{align*}
& \dot{g}_{1}=-\left(t_{1} \sin 2 g_{1}+t_{2} \cos 2 g_{1}\right),  \tag{42a}\\
& \dot{g}_{2}=t_{1} \cos 2 g_{1}-t_{2} \sin 2 g_{1},  \tag{42b}\\
& \dot{g}_{3}=2 \exp \left(-2 g_{2}\right)\left(t_{1} \sin 2 g_{1}+t_{2} \cos 2 g_{1}\right) \tag{42c}
\end{align*}
$$

Here one can see the usefulness of the basis $X_{i}$ : (i) the system of four equations is solvable; and (ii) the system (42) is decoupled. A simple transformation

$$
\begin{equation*}
h=\tan g_{1} \quad \text { or } g_{1}=\tan ^{-1} h \tag{43}
\end{equation*}
$$

transforms equation (42a) into a Riccati DE

$$
\begin{equation*}
\dot{h}=-2 t_{i} h-t_{2}\left(1-h^{2}\right), \quad \text { with } h(0)=0 . \tag{44}
\end{equation*}
$$

Having solved equation (44), one knows $g_{1}$, and equations ( $42 b, c$ ) can be solved by simple quadratures. This is the best that can be expected: the reduction of the whole problem to the solution of the Riccati DE (44).

### 3.2. Total solution

We have, putting together equations (24) with (27), (31) with (36), and (41):

$$
\begin{align*}
& Q(t)=Q_{\mathrm{R}} Q_{\mathrm{T}}=Q_{\mathrm{T}} Q_{\mathrm{R}}=Q_{\mathrm{T}} Q_{\mathrm{A}} Q_{\mathrm{S}}=Q_{\mathrm{T}}\left(\begin{array}{cc}
\cos f & \sin f \\
-\sin f & \cos f
\end{array}\right) \mathrm{e}^{\mathrm{g}_{1} X_{1}} \mathrm{e}^{\mathrm{g}_{2} X_{2}} \mathrm{e}^{\mathrm{g}_{3} X_{3}} \\
& =Q_{\mathrm{T}}\left(\begin{array}{rr}
\cos \left(f+g_{1}\right) \exp g_{2} & \cos \left(f+g_{1}\right) g_{3} \exp g_{2}+\sin \left(f+g_{1}\right) \exp \left(-g_{2}\right) \\
-\sin \left(f+g_{1}\right) \exp g_{2} & -\sin \left(f+g_{1}\right) g_{3} \exp g_{2}+\cos \left(f+g_{1}\right) \exp \left(-g_{2}\right)
\end{array}\right) \text {. } \tag{45}
\end{align*}
$$

We define new variables $\rho(t)$ and $\alpha(t)$ by (cf equation (7))

$$
\begin{equation*}
\rho \cos \alpha=y_{20} \exp \left(-g_{2}\right), \quad \rho \sin \alpha=\left(y_{10}+g_{3} y_{20}\right) \exp g_{2} \tag{46}
\end{equation*}
$$

therefore

$$
\begin{align*}
& \tan \alpha=\left(\tan \beta+g_{3}\right) \exp \left(2 g_{2}\right),  \tag{47a}\\
& \rho^{2}=y_{20}^{2} \exp \left(-2 g_{2}\right) / \cos ^{2} \alpha . \tag{47b}
\end{align*}
$$

Then, according to equation (6),

$$
\begin{equation*}
y(t)=\exp \left(\frac{1}{2} \int_{0}^{t} \operatorname{Tr} M(s) \mathrm{d} s\right) \rho(t)\binom{\sin \left(f+g_{1}+\alpha\right)}{\cos \left(f+g_{1}+\alpha\right)} . \tag{48}
\end{equation*}
$$

This result was to be expected: for $w^{2}(t)=\omega_{0}^{2}=$ constant, the solution of equation (1) is

$$
u(t)=a \cos \left(\omega_{0} t+\psi\right)
$$

A function $w=w(t)$ changes, in general, the amplitude as well as the phase into functions depending on $t$.

## 4. The WKB approximation

We start with the second parametrisation, equations (16), (17). Since $m_{2}=m_{3}$, we have exactly $f=0$, equation (35), and $Q_{\mathrm{A}}(t)=\sigma_{0}$. Van Kampen (1967) has shown that one can get the WKB approximation by neglecting the non-diagonal terms in (17). Therefore

$$
M_{\mathrm{II}} \approx\left(\begin{array}{cc}
\mathrm{i} w-\dot{w} / 2 w & 0  \tag{49}\\
0 & -\mathrm{i} w-\dot{w} / 2 w
\end{array}\right)
$$

and from equation (37)

$$
T \approx \mathrm{i} w\left(\begin{array}{rr}
1 & 0  \tag{50}\\
0 & -1
\end{array}\right)=\mathrm{i} w(t) \sigma_{3}
$$

According to theorem 1 of the Appendix we find from (33) with (75)

$$
Q_{\mathrm{S}}=\mathrm{e}^{\mathrm{ir}(t) \sigma_{3}}=\left(\begin{array}{cc}
\exp (\mathrm{ir}) & 0  \tag{51}\\
0 & \exp (-\mathrm{i} r)
\end{array}\right)=\mathrm{e}^{g_{2} X_{2}} \quad\left(g_{1}=g_{3}=0\right)
$$

where

$$
\begin{equation*}
r(t)=\int_{0}^{t} w(s) \mathrm{d} s \tag{52}
\end{equation*}
$$

Thus, with (45), for the second form of parametrisation in the WKB approximation

$$
Q=Q_{\mathrm{II}}=\left(\frac{w(0)}{w(t)}\right)^{1 / 2}\left(\begin{array}{cc}
\exp (\mathrm{i} r) & 0  \tag{53}\\
0 & \exp (-\mathrm{i} r)
\end{array}\right) .
$$

In the first form of parametrisation we obtain from (14)

$$
\begin{equation*}
Q_{\mathrm{I}}=B_{\mathrm{II}}(t) Q_{\mathrm{II}}(t) B_{\mathrm{II}}^{-1}(0), \tag{54}
\end{equation*}
$$

where $B_{\mathrm{II}}$ is given by (15). Explicitly

$$
Q_{\mathrm{I}}(t)=(w(0) w(t))^{-1 / 2}\left(\begin{array}{cc}
w(t) \cos r & -w(t) w(0) \sin r  \tag{55}\\
\sin r & w(0) \cos r
\end{array}\right)
$$

and with equation (10)

$$
\begin{equation*}
u(t)=(w(0) w(t))^{-1 / 2} \dot{u}(0) \sin r+(w(0) / w(t))^{1 / 2} u(0) \cos r . \tag{56}
\end{equation*}
$$

For the third form of parametrisation we have from (14)

$$
\begin{equation*}
Q_{\mathrm{III}}(t)=B_{\mathrm{III}}^{-1}(t) Q_{\mathrm{I}}(t) B_{\mathrm{III}}(0), \tag{57}
\end{equation*}
$$

where $B_{\text {III }}$ is given by (18). Explicitly

$$
Q_{\mathrm{III}}(t)=(w(0) / w(t))^{1 / 2}\left(\begin{array}{cc}
\cos r & -\sin r  \tag{58}\\
\sin r & \cos r
\end{array}\right)
$$

is the expression of the WKB approximation for the third form of parametrisation.
On the other hand, we have directly from $M_{\text {III }}$ in (20) $m_{2}=-w(t)=-m_{3}$; therefore, according to (35)

$$
\begin{equation*}
f(t)=-\int_{0}^{t} w(s) \mathrm{d} s=-r(t), \tag{59}
\end{equation*}
$$

and with equation (36)

$$
Q_{\mathbf{A}}(t)=\left(\begin{array}{cc}
\cos r & -\sin r  \tag{60}\\
\sin r & \cos r
\end{array}\right)
$$

From equation (27)

$$
\begin{equation*}
Q_{\mathrm{T}}(t)=(w(0) / w(t))^{1 / 2} \sigma_{0} \tag{61}
\end{equation*}
$$

Finally, according to (37), for small values of $\dot{w} / 2 w$

$$
T=-\frac{\dot{w}}{2 w}\left(\begin{array}{rr}
\cos 2 r & -\sin 2 r  \tag{62}\\
-\sin 2 r & -\cos 2 r
\end{array}\right) \approx 0
$$

Then $Q_{\mathrm{S}} \approx$ constant $=\sigma_{0}$, and $Q=Q_{\mathrm{III}}$ agrees with (58). But $Q_{\mathrm{S}}=\sigma_{0}$ implies $g_{1}=g_{2}=$ $g_{3}=0$. Therefore each set $\left\{g_{1}, g_{2}, g_{3}\right\} \neq\{0,0,0\}$ gives, in the third form of parametrisation, an improvement compared with the WKB approximation. Such a set will be calculated in the next section.

## 5. Approximate solution

We assume in equation (37) that $t_{1}$ and $t_{2}$ both contain a small factor $\epsilon$ :

$$
\begin{equation*}
t_{1}=\epsilon T_{1}, \quad t_{2}=\epsilon T_{2} \tag{63}
\end{equation*}
$$

(other cases can be discussed correspondingly). Then the series expansion

$$
\begin{equation*}
h(t)=h_{0}(t)+\epsilon h_{1}(t)+\epsilon^{2} h_{2}(t)+\ldots, \tag{64}
\end{equation*}
$$

with

$$
h_{i}(0)=0 \quad(i=0,1, \ldots),
$$

is substituted into (44). Equating coefficients of equal powers yields

$$
\begin{array}{ll}
\dot{h_{0}}=0 & \text { or } h_{0}=0 \\
\dot{h_{1}}=-T_{2} & \text { or } h_{1}=-\int_{0}^{1} T_{2}(s) \mathrm{d} s \\
\dot{h_{2}}=-2 h_{1} T_{1} & \text { or } h_{2}=2 \int_{0}^{1} \mathrm{~d} s T_{1}(s) \int_{0}^{s} \mathrm{~d} s^{\prime} T_{2}\left(s^{\prime}\right) \tag{65}
\end{array}
$$

and so on. Therefore

$$
\begin{aligned}
h(t)=-\epsilon \int_{0}^{t} & T_{2}(s) \mathrm{d} s+2 \epsilon^{2} \int_{0}^{t} \mathrm{~d} s T_{1} \int_{0}^{s} \mathrm{~d} s^{\prime} T_{2}+\ldots \\
& =-\int_{0}^{t} t_{2}(s) \mathrm{d} s+2 \int_{0}^{t} \mathrm{~d} s t_{1}(s) \int_{0}^{s} \mathrm{~d} s^{\prime} t_{2}\left(s^{\prime}\right)+\ldots
\end{aligned}
$$

In lowest order in $\epsilon$ we obtain from equation (43)

$$
\begin{equation*}
g_{1} \approx-\int_{0}^{t} t_{2}(s) \mathrm{d} s \sim \epsilon, \tag{66a}
\end{equation*}
$$

and from ( $42 b, c$ )

$$
\begin{align*}
& g_{2} \approx \int_{0}^{t} t_{1}(s) \mathrm{d} s \sim \epsilon,  \tag{66b}\\
& g_{3} \approx 2 \int_{0}^{t} t_{2}(s) \mathrm{d} s \sim \epsilon . \tag{66c}
\end{align*}
$$

The ansatz

$$
\begin{equation*}
\alpha=\beta+\gamma=\beta+\epsilon \Gamma \tag{67}
\end{equation*}
$$

where $\beta$ is given by equation (7), yields $\tan \alpha \approx \tan \beta+\gamma\left(1+\tan ^{2} \beta\right.$ ). Comparing with (47a) we get

$$
\begin{equation*}
\gamma \approx 2 y_{20}\left(y_{10} \int_{0}^{t} t_{1}(s) \mathrm{d} s+y_{20} \int_{0}^{t} t_{2}(s) \mathrm{d} s\right) /\left(y_{10}^{2}+y_{20}^{2}\right) \sim \epsilon . \tag{68}
\end{equation*}
$$

Then the total phase in equation (48) reads

$$
\begin{align*}
\phi & =f+g_{1}+\alpha=(f+\beta)+\left(g_{1}+\gamma\right)=(f+\beta)+\epsilon \ldots \\
& =(f+\beta)+\sin 2 \beta \int_{0}^{t} t_{1}(s) \mathrm{d} s+\cos 2 \beta \int_{0}^{t} t_{2}(s) \mathrm{d} s . \tag{69}
\end{align*}
$$

The main contribution comes from the antisymmetric matrix $M_{\mathrm{A}}(f)$ and from the initial conditions. The small contributions come from the symmetric, traceless matrix $M_{\mathrm{S}}$ (or $T$ ). The matrix $M_{\mathrm{T}}$ with non-vanishing trace does not influence the phase at all.

For the factor $\rho(t)$ in the amplitude of equation (48) we get now from (47b)

$$
\begin{equation*}
\rho(t)=\rho_{0}\left(1-\cos 2 \beta \int_{0}^{t} t_{1}(s) \mathrm{d} s+\sin 2 \beta \int_{0}^{t} t_{2}(s) \mathrm{d} s\right) . \tag{70}
\end{equation*}
$$

Contributions to $\rho$ come from the initial conditions ( $\rho_{0}$ and $\beta$ ) and from the symmetric, traceless matrix $M_{\mathrm{s}}$. Finally, the matrix $M_{\mathrm{T}}$ with non-vanishing trace also contributes to the total amplitude.

Equations (69) and (70) can be simplified by the definitions
$\rho_{1}(t) \cos \delta(t)=\int_{0}^{t} t_{1}(s) \mathrm{d} s, \quad \rho_{1}(t) \sin \delta(t)=\int_{0}^{t} t_{2}(s) \mathrm{d} s, \quad \rho_{1} \sim \epsilon$.
Then

$$
\begin{equation*}
\phi=(f+\beta)+\rho_{1}(t) \sin (2 \beta+\delta(t)), \quad \rho(t)=\rho_{0}\left[1-\rho_{1}(t) \cos (2 \beta+\delta(t))\right] . \tag{72}
\end{equation*}
$$

## Appendix. Some elementary matrix algebra

Theorem 1. Given the matrix DE $\dot{Z}(t)=K(t) Z(t)$ with $Z(0)=I$ and $K(t)$ analytic in $I_{t}$, then a solution of the form

$$
Z(t)=\exp \left(\int_{0}^{t} K(s) \mathrm{d} s\right)
$$

exists, if and only if the commutator

$$
\left[K(t), \int_{0}^{t} K(s) \mathrm{d} s\right]=0
$$

for all $t \in I_{t}$. For a proof see, for example, Martin (1968).
For the Pauli matrices we use the following representation:
$\sigma_{0}=\left(\begin{array}{ll}1 & 0 \\ 0 & 1\end{array}\right), \quad \sigma_{1}=\left(\begin{array}{ll}0 & 1 \\ 1 & 0\end{array}\right), \quad \sigma_{2}=\left(\begin{array}{rr}0 & -\mathrm{i} \\ \mathrm{i} & 0\end{array}\right), \quad \sigma_{3}=\left(\begin{array}{rr}1 & 0 \\ 0 & -1\end{array}\right)=X_{2}$.

Then

$$
X_{1}=\mathrm{i} \sigma_{2}=\left(\begin{array}{rr}
0 & 1  \tag{73}\\
-1 & 0
\end{array}\right), \quad X_{3}=\sigma_{+}=\left(\sigma_{1}+\mathrm{i} \sigma_{2}\right) / 2=\left(\begin{array}{ll}
0 & 1 \\
0 & 0
\end{array}\right) .
$$

We need the exponentials (defined as $\mathrm{e}^{A}=\Sigma_{n=0}^{\infty} .4^{n} / n!$ )

$$
\begin{align*}
& \mathrm{e}^{\alpha X_{2}}=\exp \left(\begin{array}{cc}
\alpha & 0 \\
0 & -\alpha
\end{array}\right)=\left(\begin{array}{cc}
\exp \alpha & 0 \\
0 & \exp (-\alpha)
\end{array}\right),  \tag{75}\\
& \mathrm{e}^{\alpha X_{3}}=\sigma_{0}+\alpha X_{3}=\left(\begin{array}{ll}
1 & \alpha \\
0 & 1
\end{array}\right), \quad \text { since } X_{3}^{2}=0 . \tag{76}
\end{align*}
$$

$\mathrm{e}^{\alpha X_{1}}$ can also be calculated by a series expansion, or, with

$$
P=\left(\begin{array}{rr}
1 & -1 \\
\mathrm{i} & \mathrm{i}
\end{array}\right) \quad \text { and } D=\left(\begin{array}{rr}
\mathrm{i} & 0 \\
0 & -\mathrm{i}
\end{array}\right)
$$

as follows:

$$
\begin{gather*}
\mathrm{e}^{\alpha X_{1}}=\exp \left(\alpha P D P^{-1}\right)=\dot{P} \mathrm{e}^{\alpha D} P^{-1}=P\left(\begin{array}{cc}
\exp (\mathrm{i} \alpha) & 0 \\
0 & \exp (-\mathrm{i} \alpha)
\end{array}\right) P^{-1} \\
=\left(\begin{array}{cc}
\cos \alpha & \sin \alpha \\
-\sin \alpha & \cos \alpha
\end{array}\right)=\sigma_{0} \cos \alpha+X_{1} \sin \alpha \tag{77}
\end{gather*}
$$

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