

RULES FOR MATRIX ELEMENT EVALUATIONS IN JWKB APPROXIMATION*

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Using the properties of the so-called fundamental solutions to the one-dimensional Schroedinger equation having Fröman and Fröman form the rules are formulated which allow one to evaluate matrix elements in the JWKB approximation and its generalizations. The rules apply to operators $M(x, d/dx)$, M being polynomial functions of their arguments. The applicability of the rules depends on the properties of the so-called canonical indices introduced in this paper. The canonical indices are global characteristics of underlying Stokes graphs. If sufficiently small in comparison with unity they allow one to apply safely the JWKB approximation within the so-called ε -reduced canonical domains of a given Stokes graph. The 0th canonical index for the n th energy level Stokes graph corresponding to the harmonic oscillator potential is found to be $\varepsilon^{\text{CAN}} = 0.678/(2n+1)$. If the application of the rules is allowed then approximated matrix elements are obtained in an unambiguous way and with an accuracy controlled by corresponding canonical indices. Several examples of matrix elements are considered to illustrate how the rules should be used. Limitations to the rules are also discussed with the aid of suitably chosen examples.

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1. Introduction

Evaluation of matrix elements with the help of the JWKB approximations is one of their main applications in quantum mechanics (see, for example, Landau and Lifshitz [1] and Fröman and Fröman [2, 4, 15] and the references quoted in the latter reference). A modern use of the JWKB approximations (generalized to the form of the phase-integral approximations [3, 8, 9]) to evaluate one-dimensional matrix elements has been originated by Fröman and Fröman [4]. The authors have given simple and elegant formulae for calculating one-dimensional matrix elements for a single-well potential in the JWKB as well as in the higher order phase-integral approximations.

However, still new modifications are being introduced to the method in order to improve its accuracy. Recently, Streszewski and Jędrzejek [5] have evaluated the non-orthogonal matrix elements in the JWKB approximation using the Feynman path integral formalism. They found that the integration prescription given by Fröman and Fröman [4]

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had to be modified in some cases and these modifications greatly improved numerical results for the potentials considered by the authors both in the case when the JWKB approximation was used and in the case when the method was generalized to include the higher order phase integral approximations.

A by-product of the Streszewski and Jędrzejek paper [5] is a conclusion that the Fröman and Fröman formula [4] cannot be considered as a general rule for matrix element calculations in the JWKB approximation. On the other hand, operating with the JWKB approximations themselves one cannot infer what is the proper way of using them in integrations. This is, as it seems, why Streszewski and Jędrzejek used the Feynman path integral for their studies of the JWKB approximated integrals. The Feynman path integral method itself is surely as reliable as simple enough to obtain the proper results for sufficiently simple matrix elements at the JWKB level. But one can hardly imagine its effective application to calculate more complicated matrix elements (for example, in the case of many-well potentials) or when higher order phase-integrals [3] or generalized JWKB approximations [6] are to be used. On the other hand it would be desirable to have some general rules for evaluating a sufficiently arbitrary matrix element to an arbitrary order of the approximation chosen and with controlled and good accuracy.

It is the goal of the paper to formulate such rules.

The starting point of our analysis leading to the rules are the exact solutions to the Schroedinger equations found by Fröman and Fröman [3].

From infinitely many solutions to the Schroedinger equation having the Fröman and Fröman form we select finite sets of them called fundamental solutions and defined in Appendix 1 and we use them in a way formulated there (see also our earlier papers [6, 14]).

The fundamental solutions can be given forms appropriate for the approximations actually used i.e. the forms of the phase integral approximation [3, 8, 9] or of the generalized JWKB formula [6] or simply the form of the conventional JWKB formula (see A1.17) in Appendix 1)¹.

The fundamental solutions and their properties play the main role in the formulation of the rules. In order to describe this role properly we have introduced a number of notions, such as JWKB points of the fundamental solutions, their canonical points and canonical domains, their ε -reduced canonical domains and ε -reduced Stokes graph, a JWKB approximation allowing Stokes graph, a canonical index of the Stokes graph and so on, in terms of which we have described the properties of the fundamental solutions relevant for establishing the rules.

All the notions mentioned above, the properties of the fundamental solutions and the way of using them as well as all other key facts about the fundamental solutions and their JWKB approximations relevant for the subject considered in the paper have been gathered in Appendix 1. We have also formulated there a necessary and sufficient condition for a global application of the JWKB approximation (i.e. in the whole area of the

¹ In what follows we shall use a phrase "the JWKB approximation" in the sense defined by (A1.14) which covers all the cases cited above (see (A1.17)).

ε -reduced Stokes graph). Therefore, the content of Appendix 1 should be regarded rather as an essential introduction to the subject of the paper and acquainting with it seems to be necessary (and sufficient) for understanding the basis on which the rules are formulated on.

Safe applications of the rules call for checking that the conditions allowing such applications are indeed fulfilled (see formulae (A1.19) and (A1.21) in Appendix 1). But it is usually difficult to perform such a check explicitly (i.e. to find explicit forms of the relevant canonical indices) and one is often left only with a belief that if performed the check would be positive. Therefore, in such cases the approximations obtained from the rules should be regarded rather as the optimum i.e. as the best ones if the JWKB approximations for the wave functions are to be used at all.

The paper is organized as follows.

In Section 2 the rules are formulated in general.

In Section 3 particular examples of nonorthogonal matrix elements between bound-bound states in the simplest case of the one-well potential are investigated. The aim of this Section is to show how the rules work as well as to compare our results with those obtained earlier by Fröman and Fröman [4] and by Streszewski and Jędrzejek [5].

In Section 4 more general cases of nonorthogonal matrix elements between bound and unbound states are investigated in the presence of an additional potential well without bound states.

In Section 5 we show how the rules can be applied when the generalized JWKB formulae are used as the approximations.

The results obtained in Sections 3–5 assume that all the Stokes graphs relevant for the considerations are the JWKB approximation allowing graphs (in the sense defined in Appendix 1). This assumption allows to apply the rules safely.

Limitations to the rules are considered in Section 6. They arise when necessary conditions for the rules to be applied are broken. This happens when some relevant pairs of turning points are not canonically well separated (see Appendix 1 for definition). In some of such cases the approximate JWKB integrations can be performed by breaking some of the rules. In some others the JWKB approximations cannot be used at all. An example of this situation is provided by the supersymmetric quantum mechanics [7, 10–12].

The results of the paper are summarized in Section 7 where some conclusions are also drawn.

2. The rules

The rules we are going to formulate are limited to approximate calculations of matrix elements containing quantities of the following type:

$$M(x, d/dx) = \sum_{k=0}^n M_k(x) d^k / a x^k, \quad (2.1)$$

where $M_k(x)$, $k = 0, 1, \dots, n$, are rational functions of x holomorphic in some vicinity of the real axis. Such an assumption allows the asymptotic properties of $M_k(x)$ for $x \rightarrow \infty$,

$k = 0, 1, \dots, n$, not to be taken into account if the JWKB approximation of the relevant matrix elements is considered. On the other hand necessary properties of the derivatives of the fundamental solutions and their JWKB approximations have been considered in Appendix 1 (see A1.6).

The following is the Basic Assumption for our further considerations in this and in the next Sections (see Appendix 1 A1.4–A1.5 for relevant definitions): *Each Stokes graph is the JWKB approximation allowing graph.*

As we have shown in Appendix 1 the above assumption is equivalent to the statement that the turning points of each considered Stokes graph are canonically well separated or that canonical indices of the graphs are much smaller than unity. Especially the latter quantities seem to be extremely useful in practice since if known they allow us to estimate whether the relevant calculations using the JWKB approximations can be performed at all and, if so, with what accuracy.

Usually, the canonical indices are not easy to obtain. To illustrate, however, their usefulness we have calculated the lowest (0th) canonical index for the harmonic oscillator to get for the n th energy level Stokes graph: $\epsilon^{\text{CAN}} = 0.678/(2n+1)$. It is seen that in the case of the harmonic oscillator the JWKB approximations should give good results already for, say, $n \geq 5$.

The above Basic Assumption allows us in principle to use the JWKB approximations $C_r \psi_{D_k}^{\text{JWKB}}$, $r = 0, 1, \dots, n$, $k = 1, \dots, p$, and the corresponding ϵ_n^{CAN} —reduced Stokes graph S_c^n in the same way as the fundamental solutions ψ_{D_k} , $k = 1, \dots, p$, themselves are used together with their derivatives and with the Stokes graph S that corresponds to them.

However, operating with ψ_{D_k} 's or their derivatives one must sometimes to appeal to their holomorphicity at each turning point—the property which is not shared by any of their approximations $C_r \psi_{D_k}^{\text{JWKB}}$. Therefore, to avoid possible confusions in such cases as well as to have a clear insight into which operations and formulae are approximated and which are exact we prefer to operate originally with ψ_{D_k} 's making the desired JWKB approximations only in the final steps.

We are now ready to formulate the first basic rule for matrix element calculations in the JWKB approximations:

(i) *Keep the integration contour running through the canonical domains of the fundamental solutions used to represent the physical wave functions in the matrix element integral (s).*

However, the rule (i) although basic is far from being sufficient for writing unambiguously the desired approximation to the integral considered. In fact, we are faced with the following situation:

a) there are many different but equivalent, exact integral formulae fulfilling the rule (i) and representing the same matrix element;

b) the formulae differ by sets of the fundamental solutions they use as well as by contours of integrations;

c) in different formulae their integrands can differ by their dominant behaviour in the same canonical domains through which the integration contours run.

It should be clear, however, that the best JWKB approximation for the considered matrix element should be provided by the formulae which offers the weakest dominant behaviour of their integrands when the integration runs through the corresponding canonical domains. Such integral formulae will be called dominant integral representations for the matrix element considered.

On the other hand, the integral formulae with a stronger dominant behaviour of their integrands should vanish if JWKB approximated since, otherwise, they would provide stronger dominant contributions to the considered matrix element than it is allowed by the property of the latter. Such integral representations for a given matrix element will be called 'overdominating' representations.

Therefore, the following next rule should be applied when the JWKB approximation is used:

(ii) *Choose the integral formulae offering the weakest dominant behaviour of their integrands in the same canonical domains.*

Nevertheless, both the above rules do not fix uniquely the ways of integrating with the JWKB approximations.

A further selection of the best approximate integral formula can be done by analysing the behaviour of its integrand at different regions of the real axis, when the integration contour is deformed so as to run along the real axis (but passing, of course, above (or below) classical turning points). Thus, for example, if some particular regions of the real axis are classically forbidden for one (or both) of the integrated wave functions, the function(s) should increase (or decrease) exponentially in such regions when x increases along the axis. Therefore, if the integrand of the approximate formula resulting from the chosen integral representation for the considered matrix element behaves improperly in the relevant regions of the real axis then such an approximate formula should be eliminated in favour of its alternatives.

Similarly, a proper behaviour of the integrand in the classically allowed regions should guide us in making the proper choice between appearing possibilities.

Therefore, the next rule can be formulated as follows:

(iii) *From varieties of possible approximate formulae choose the one with the proper behaviour of its integrand (s) at classically forbidden as well as at classically allowed regions.*

The rules (i)–(iii) formulated above are now sufficient for obtaining in a unique way the JWKB approximation for an arbitrary matrix element involving a quantity of the type (2.1).

Let us note, however, that effective applications of the rules (i)–(iii) have to assume that energy levels labelling the integrated wave functions have also been quantized with the help of the corresponding fundamental solutions and the relevant quantization has been performed in accordance with the rules (i)–(iii).

First of all it means that a necessary procedure of matching different fundamental solutions has been performed in accordance with the condition that each fundamental solution involved in the procedure has not left its canonical domain. As it follows from Appendix 1 this condition can always be satisfied.

The quantization condition can be then approximated according to our Basic Assumption and used in approximate integrations of the corresponding matrix elements.

It means further that the accuracies of both the approximations are strictly related: one cannot expect a good JWKB approximation for integrals if it appears unsatisfactory for quantization conditions.

It seems, however, that in general it is easier to satisfy the relevant conditions when applying the JWKB approximation to quantize energy levels than to calculate the relevant matrix elements. In fact, the rules (i)–(iii) seem to exclude the existence of any good JWKB approximation for some particular matrix elements even if the corresponding quantization conditions can be obtained without troubles. A relevant example is considered in Section 6.

3. Nonorthogonal matrix elements between bound-bound states

We are going to consider now so-called non-orthogonal matrix elements (see, for example, Streszewski and Jędrzejek [5]). Such elements are labeled by energy eigenvalues of two, in general different, hamiltonians. Therefore, Stokes graphs corresponding to each energy are independent and can differ essentially from each other. In particular, relative positions of sets of their turning points can be also arbitrary.

If the matrix elements corresponding to the case are to be JWKB approximated then not all relative positions of the relevant Stokes graphs are allowed. The allowed positions are those which satisfy the following condition:

It is possible to deform the integration contour in a way being not only in accordance with the rules (i)–(iii) of Section 2 applied to each (of the two) ε -reduced Stokes graph separately but also in such a way that none of the 'holes' (of any of the two ε -reduced Stokes graphs) lying on one side of the integration contour overlaps any 'hole' lying on the other side of the contour.

It is assumed that this condition is satisfied in this and in Sections 4 and 5. This assumption allows us to use rather the Stokes graphs themselves than the corresponding ε -reduced graphs to characterize cases we are going to consider.

Let $\psi_1(x)$ and $\psi_2(x)$ be the normalized eigenfunctions (with respective eigenvalues E_1 and E_2) corresponding to the hamiltonians H_1 and H_2 defined by the single — well potentials $V_1(x)$ and $V_2(x)$, respectively. We shall consider the following matrix element:

$$M_{12} = \int_{-\infty}^{+\infty} \psi_1(x) M(x, d/dx) \psi_2(x) dx, \quad (3.1)$$

where $M(x, d/dx)$ has the form (2.1).

3.1. Nested position of classical regions

As the first example of (3.1) we investigate the one corresponding to Fig. 1 which shows the relative position of the potentials V_1 and V_2 . To evaluate M_{12} using the fundamental solution representations for $\psi_1(x)$ and $\psi_2(x)$ we have to deform the integration

contour in (3.1) from the x -axis going around the classical turning points $a_k, b_k, k = 1, 2$, which are singular for the corresponding functions $\omega_k(x), k = 1, 2$, defining the fundamental solutions (A1.7).

For the time being we shall limit our considerations to the JWKB approximations defined by the cases 1 and 2 of the formula (A1.17). The case 3 will be discussed later (see Section 5).

Let Fig. 2 represent the Stokes graphs corresponding to Fig. 1. We deform the integration contour in (3.1) in the way shown in Fig. 2 where the points A_L and A_R are taken at the boundaries of the 'holes' of the ε -reduced Stokes graph $S_{1\varepsilon}$ corresponding to the graph S_1 (solid lines in Fig. 2), i.e. we have:

$$M_{12} = \left(\int_{-\infty}^{A_L} + \int_K + \int_{A_R}^{+\infty} \right) \psi_1(x) M(x, d/dx) \psi_2(x) dx. \quad (3.2)$$

According to the rules (i)–(iii) of Section 2 we should substitute now $\psi_1(x)$ and $\psi_2(x)$ by their corresponding fundamental solution representations (defined by the Stokes graphs of Fig. 2) for which the points of the integration contour in (3.2) are canonical. The sets of the fundamental solutions relevant for the case are: $\{\psi_{k,L}, \psi_{k,R}, \psi_{k,U}, \psi_{k,D}\}, k = 1, 2$.

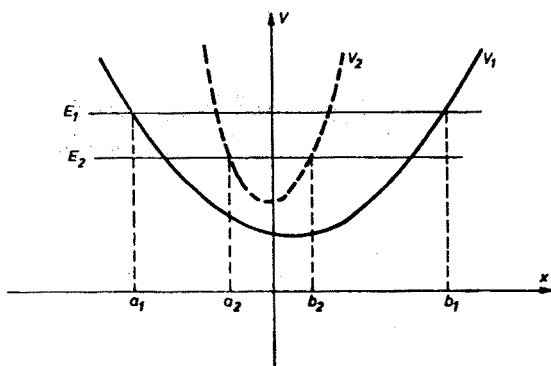


Fig. 1. The nested position of the potentials V_2 and V_1

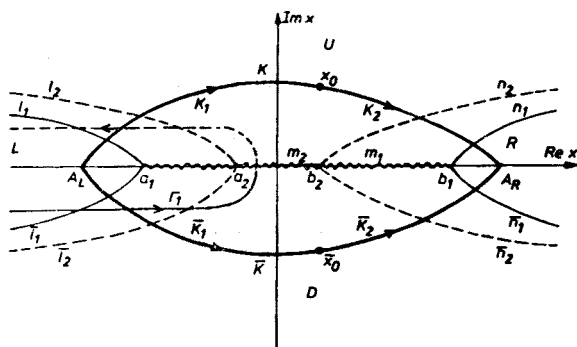


Fig. 2. The Stokes graph corresponding to Fig. 1

TABLE I

Canonical domains	Boudnaries
$D_{k,L}$	m_k, n_k, \bar{n}_k
$D_{k,R}$	l_k, \bar{l}_k, m_k
$D_{k,U}$	\bar{l}_k, \bar{n}_k
$D_{k,D}$	l_k, n_k

We have of course $\psi_k \equiv C_{k,L} \psi_{k,L} \equiv C_{k,R} \psi_{k,R}$ (see Appendix 2) where $C_{k,L}$ and $C_{k,R}$, $k = 1, 2$, are some normalization constants and the equations $C_{k,L} \psi_{k,L}(x) \equiv C_{k,R} \psi_{k,R}(x)$ mean the quantization conditions for the energies E_k , $k = 1, 2$.

The canonical domain $D_{k,X}$ for the respective solution $\psi_{k,X}$, $k = 1, 2$, $X = L, R, U, D$ contains the sectors X where the solution is defined and is bounded by the corresponding Stokes' lines given in Table I.

Therefore, according to our Basic Assumption we should make the following replacement in the first and third integrals in (3.2):

$$\psi_1(x) \rightarrow \begin{cases} C_{1,L} \psi_{1,L}^{\text{JWKB}}(x), & x \in (-\infty, A_L), \\ C_{1,R} \psi_{1,R}^{\text{JWKB}}(x), & x \in (A_R, +\infty), \end{cases}$$

and

$$M(x, d/dx) \psi_2(x) \rightarrow \begin{cases} C_{2,L} M_{\text{mod}} \psi_{2,L}^{\text{JWKB}}(x), & x \in (-\infty, A_L), \\ C_{2,R} M_{\text{mod}} \psi_{2,R}^{\text{JWKB}}(x), & x \in (A_R, +\infty), \end{cases} \quad (3.3)$$

where:

$$M_{\text{mod}}(x) = \sum_{k=0}^n M_k(x) C_k^\sigma(x), \quad (3.4)$$

with $C_k^\sigma(x)$, $k = 0, 1, \dots, n$, defined by (A1.33).

However, the second integral in (3.2) can be represented at least in two ways. First, the integration along K can be broken at the point x_0 into two parts (see Fig. 2) and then we can make analogous substitutions as follows:

$$\begin{aligned} \int_{K_1} [\psi_1 M \psi_2]^{\text{JWKB}} dx &= C_{1,L} C_{2,L} \int_{K_1} \psi_{1,L}^{\text{JWKB}} M_{\text{mod}} \psi_{2,L}^{\text{JWKB}} dx, \\ \int_{K_2} [\psi_1 M \psi_2]^{\text{JWKB}} dx &= C_{1,R} C_{2,R} \int_{K_2} \psi_{1,R}^{\text{JWKB}} M_{\text{mod}} \psi_{2,R}^{\text{JWKB}} dx. \end{aligned} \quad (3.5)$$

Let us now take the following representations for the JWKB factors $\psi_{r,X}^{\text{JWKB}}$ of the fundamental solutions $\psi_{r,X}$, $r = 1, 2$, $X = L, R, U, D$:

$$\begin{aligned} \psi_{r,L}^{\text{JWKB}}(x) &= iQ_r^{-1/4}(x) \exp[-i w_r(x)], \\ \psi_{r,U}^{\text{JWKB}}(x) &= Q_r^{-1/4}(x) \exp[+i w_r(x)], \end{aligned}$$

$$\begin{aligned}\psi_{r,D}^{\text{JWKB}}(x) &= \psi_{r,U}^{\text{JWKB}}(x), \\ \psi_{r,R}^{\text{JWKB}}(x) &= Q_r^{-1/4}(x) \exp[-iv_r(x)], \quad r = 1, 2,\end{aligned}\quad (3.6)$$

with $iw_r(x) = \int_{a_r}^x Q_r^{1/2} dy$ defined in the x -plane with the cut along the line $(a_r, +\infty)$ and with $iv_r(x) = \int_{b_r}^x Q_r^{1/2} dy$ and the corresponding cut at $(-\infty, b_r)$. Taking also into account the approximate quantization conditions: $iC_{k,L} = \exp[+iw_k(b_k)]C_{k,R}$, $k = 1, 2$ (see Appendix 2) we get for M_{12}^{JWKB} :

$$M_{12}^{\text{JWKB}} = -C_{1L}C_{2L}\left(\int_{-\infty}^{A_L} + \int_K + \int_{A_R}^{+\infty}\right)(Q_1Q_2)^{-1/4} \exp[-i(w_1+w_2)]M_{\text{mod}}dx. \quad (3.7)$$

In the second way of the integration we can write:

$$\int_K \psi_1 M \psi_2 dx = C_{1,L} \int_K (\alpha_{1,L} \psi_{1,U} + \bar{\alpha}_{1,L} \psi_{1,D}) M_{\text{mod}} \psi_2 dx, \quad (3.8)$$

where $\alpha_{1,L} \equiv \alpha_{1,L/U \rightarrow D}$ is the canonical coefficient obtained with the aid of (A1.16).

Next, we perform the integration in the second term ($\equiv I_2$) in (3.8) by deforming K into \bar{K} (a path complex conjugate to K) and after that we repeat the procedure of replacing the fundamental solutions by their JWKB approximations as follows (note that $\alpha_{1,L}^{\text{JWKB}} = 1$, see Appendix 2):

$$\begin{aligned}I_2 &= \int_K (\alpha_{1,L} \psi_{1,U} + \bar{\alpha}_{1,L} \psi_{1,D}) M \psi_2 dx = \alpha_{1,L} \int_K \psi_{1,U} M \psi_2 dx \\ &\quad + \bar{\alpha}_{1,L} \int_{\bar{K}} \psi_{1,D} M \psi_2 dx\end{aligned}$$

and

$$\begin{aligned}I_2^{\text{JWKB}} &= \{iC_{2,L} \int_{K_1} + C_{2,R} \exp[+iw_2^+(b_2)] \int_{K_2}\} (Q_1Q_2)^{-1/4} \exp[+i(w_1-w_2)] M_{\text{mod}} dx \\ &\quad - \{iC_{2,L} \int_{\bar{K}_1} + C_{2,R} \exp[+iw_2^+(b_2)] \int_{\bar{K}_2}\} (Q_1Q_2)^{-1/4} \exp[+i(w_1-w_2)] M_{\text{mod}} dx \\ &= iC_{2,L} \int_{\Gamma} (Q_1Q_2)^{-1/4} \exp[+i(w_1-w_2)] M_{\text{mod}} dx,\end{aligned}\quad (3.9)$$

where $\Gamma = K - \bar{K}$ ($-\bar{K}$ means the integration along \bar{K} in the opposite direction) and $w_i^\pm(b_i)$, $i = 1, 2$, mean the corresponding values taken above (+) or below (—) the cuts. Let us note that the deformation of K into \bar{K} in (3.9) is allowed since the functions $\psi_{1,D}$ and ψ_2 are holomorphic in each classical turning point. Also each substitution: $\psi \rightarrow \psi^{\text{JWKB}}$ has been performed in the canonical domains of the corresponding fundamental solutions. We get finally for M_{12}^{JWKB} :

$$\begin{aligned}M_{12}^{\text{JWKB}} &= -C_{1,L}C_{2,L}\left(\int_{-\infty}^{A_L} + \int_{A_R}^{+\infty}\right)(Q_1Q_2)^{-1/4} \exp[-i(w_1+w_2)] M_{\text{mod}} dx \\ &\quad + iC_{1,L}C_{2,L} \int_{\Gamma} (Q_1Q_2)^{-1/4} \exp[+i(w_1-w_2)] M_{\text{mod}} dx.\end{aligned}\quad (3.10)$$

Both the formulae (3.7) and (3.10) fulfil the rules (i) and (iii). But they differ of course by the behaviour of their integrands in the domains $D_{k,U}$ and $D_{k,D}$, $k = 1, 2$. (Note, that the integration in (3.7) along K can be substituted by the integration along \bar{K} with the same integrand). The behaviour of the integrand in the second integral in (3.7) is dominant in the domains $D_{k,X}$, $k = 1, 2$, $X = D, U$, in comparison with the corresponding integrand in (3.10) (the integration along $\Gamma = K - \bar{K}$). To see this let us take any point x in the sector U such that $x \in V_{e,U} \equiv U \cap K_{1e,L}^{\text{CAN}(n)} \cap K_{1e,U}^{\text{CAN}(n)} \cap K_{1e,D}^{\text{CAN}(n)}$. In each of such points the solutions $\psi_{1,X}$, $X = L, U, D$, can be approximated by their JWKB factors (3.6) since the conditions (A1.22) are fulfilled for such x (by our Basic Assumption). However, for the points x we also have $\psi_{1,L} = \alpha_{1,L}\psi_{1,U} + \bar{\alpha}_{1,L}\psi_{1,D}$ and hence $\psi_{1,L}^{\text{JWKB}} = \alpha_{1,L}\psi_{1,U}^{\text{JWKB}} + \bar{\alpha}_{1,L}\psi_{1,D}^{\text{JWKB}}$. But, when $x \in V_{e,U}$ then $\psi_{1,L}^{\text{JWKB}} = \psi_{1,D}^{\text{JWKB}} = iQ^{-1/4}(x) \exp[-i w_r(x)]$ and $\psi_{1,U}^{\text{JWKB}}$ has to be only an ε^{CAN} -part of $\psi_{1,D}^{\text{JWKB}}$ and also of $\psi_{1,L}^{\text{JWKB}}$ in $V_{e,U}$ i.e. $|\psi_{1,U}^{\text{JWKB}}| < \varepsilon^{\text{CAN}} |\psi_{1,L}^{\text{JWKB}}|$ for $x \in V_{e,U}$. Therefore, the integrand in the last integral in (3.10) is also an ε^{CAN} -part of the corresponding integrand of the middle integral in (3.7). But the integrations along K in (3.7) and along Γ in (3.10) define the same integral the order of which has therefore to be determined by the last term in (3.10). This is in fact what the rule (ii) says. Therefore, the accepted formula has to be (3.10) and the middle 'overdominating' integral in (3.7) has to vanish (see the example discussed by Fröman and Fröman [4]).

The formula (3.10) is well known and was first obtained by Fröman and Fröman [4] (see also Streszewski and Jędrzejek [5]) who also considered its alternative obtained by the permutation $1 \leftrightarrow 2$ of the indices in (3.10) since M_{12} is symmetric under such operation. However, the *approximation* (3.10) changes under the permutation since the Stokes graphs in Fig. 2 are *not* symmetric under the exchange $1 \leftrightarrow 2$. Therefore, the new formula obtained in this way is indeed different from (3.10). However, it cannot be better and in fact it is excluded by the rule (iii). To see this we should note that we can perform the desired integrations in (3.10) just along the cut (a_1, b_1) in both the cases, deforming properly the closed contour Γ . However, the function $\exp[-i w_2(x)]$ in (3.10) increases and decreases exponentially at the segments (a_1, a_2) and (b_2, b_1) of the cut, respectively, if x increases through the segments. Such a behaviour is expected and correct since these segments are classically forbidden regions. On the other hand, the behaviour would be quite opposite i.e. wrong for the function $\exp[+i w_2(x)]$ which would appear in (3.10) after the permutation.

There are possible yet similar mutations of the formula (3.10). However, all of them are excluded due to the wrong behaviour of their integrands in classically forbidden regions.

Let us note further that the normalization constants $C_{1,L}$ and $C_{2,L}$ can be readily obtained from (3.8) by putting there $V_1 \equiv V_2$, $M \equiv 1$ and $M_{12}^{\text{JWKB}} = 1$.

Finally, the accuracy of the approximation (3.10) can be estimated with the help of the full series (A1.8) (see Appendix 2). The measure of this accuracy (see (A2.5)) depends explicitly on the energy levels labelling the matrix elements M_{12} . This is in contrast with the form of the approximation (3.9) itself suggesting the insensitivity of its accuracy to the energy levels. In fact, as it follows from (A2.5), the accuracy of (3.9) should be the worse the lower energy levels label M_{12} .

3.2. Overlapping classical regions

As a second example of the matrix element (3.1) let us consider the case defined by Fig. 3 (the case (b) of the Streszewski and Jędrzejek paper [5]). The canonical domains $D_{k,X}$ for the relevant solutions $\psi_{k,X}$, $k = 1, 2$, $X = L, R, U, D$, remain, of course, unchanged (see Table I). However, we cannot apply readily the formula (3.10) to the case since it causes $\exp[iw_1(x)]$ to increase at the segment (b_1, b_2) i.e. to behave incorrectly there. Therefore, to obtain the properly approximated integrand in (3.2) we should integrate according to Fig. 4 to get:

$$\begin{aligned} \int_K \psi_1 M \psi_2 dx = & C_{1,L} C_{2,L} [\alpha_{1,L} \int_{A_L}^{x_1} \psi_{1,U} M \psi_{2,L} dx + \alpha_{1,L} \bar{\alpha}_{2,L} \int_{x_1}^B \psi_{1,U} M \psi_{2,D} dx] \\ & + \alpha_{1,L} \alpha_{2,L} C_{1,L} C_{2,L} \int_B^{x_2} \psi_{1,D} M \psi_{2,U} dx + C_{1,R} C_{2,L} \alpha_{2,L} \int_{x_2}^{A_R} \psi_{1,R} M \psi_{2,U} dx \\ & + C_{1,L} C_{2,L} [\bar{\alpha}_{1,L} \int_{A_L}^{\bar{x}_1} \psi_{1,D} M \psi_{2,L} dx + \bar{\alpha}_{1,L} \alpha_{2,L} \int_{\bar{x}_1}^B \psi_{1,D} M \psi_{2,U} dx] \\ & + \alpha_{1,L} \bar{\alpha}_{2,L} C_{1,L} C_{2,L} \int_B^{\bar{x}_2} \psi_{1,U} M \psi_{2,D} dx + C_{1,R} C_{2,L} \bar{\alpha}_{2,L} \int_{x_2}^{A_R} \psi_{1,R} M \psi_{2,D} dx \\ & + 2\text{Re}\{\alpha_{1,L} \alpha_{2,L} C_{1,L} C_{2,L} \int_{x_1}^{x_2} \psi_{1,U} M \psi_{2,U} dx\}. \end{aligned} \quad (3.11)$$

The above expression is *exact*. According to our Basic Assumption all the fundamental solutions present in each of the integrands in (3.11) can be substituted now by its corresponding JWKB approximation. However, we can first get rid of the last term in (3.11) putting $x_1 = x_2$ in it. Making this and the desired JWKB substitutions as well as using, as usual, the approximate quantization conditions we get:

$$\int_K [\psi_1 M \psi_2 dx]^{\text{JWKB}} = i C_{1,L} C_{2,L} \int_{K'} (Q_1 Q_2)^{-1/4} \exp[+i(w_1 - w_2)] M_{\text{mod}} dx, \quad (3.12)$$

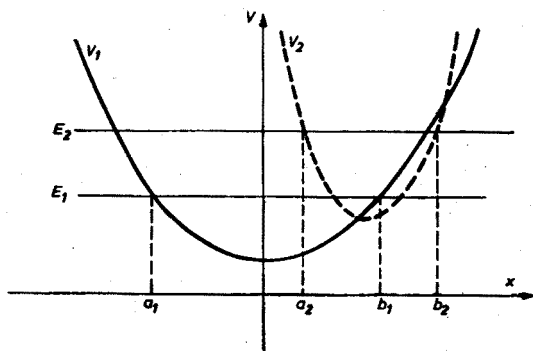


Fig. 3. The potentials V_1 and V_2 with overlapping classical regions

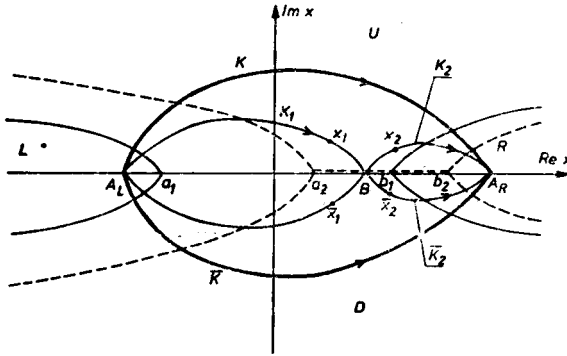


Fig. 4. The Stokes graph corresponding to Fig. 3

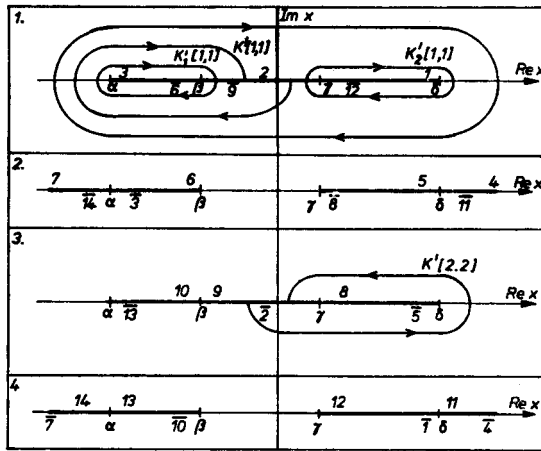


Fig. 5. The Riemann surface of $(Q_1Q_2)^{-1/4}$ with the integration contours corresponding to the cases shown in figures 1-6

where the contour K' is closed in the corresponding Riemann surfaces for the functions $(Q_1Q_2)^{-1/4}$, $Q_k^{1/2}$, $k = 1, 2$. The Riemann surface for $(Q_1Q_2)^{-1/4}$ is shown in Fig. 5 (where K' is shown as the solid line). On the surfaces the integrand in (3.12) is the uniquely defined function if the approximate quantization conditions $\int_{\Gamma_k} Q_k^{1/2} = (2n+1)\pi i$, $k = 1, 2$ are also taken into account (Γ_k runs around the cut (a_k, b_k) clockwise). The Riemann surface for $(Q_1Q_2)^{-1/4}$ consists of the four cut x -planes (numbered from 1. to 4. in the figure) which are sewed along the edges carrying the same numbers (n — for the upper edges and \bar{n} — for the bottom ones). The Riemann surfaces for the functions $Q_k^{1/2}$, $k = 1, 2$, are obtained by cutting the x -plane along the segments (a_k, b_k) , $k = 1, 2$, correspondingly. For the case just considered we should put in the figure: $\alpha = a_1$, $\beta = a_2$, $\gamma = b_1$, $\delta = b_2$. Only two of the sheets in Fig. 5 (i.e. 1. and 3.) are needed to close the contour K' .

Let us note, however, that in the previous case of the integration, formula (3.9), it was sufficient to consider only the first sheet of the Riemann surface in Fig. 5 (where the

points $\alpha, \beta, \gamma, \delta$ should be then identified as $\alpha = a_1, \beta = a_2, \gamma = b_2$ and $\delta = b_1$). The corresponding contour Γ is also indicated.

The Riemann surfaces for $Q_i^{1/2}, i = 1, 2$, have similar structure and are obtained by cutting the x -plane along the segments $(a_i, b_i), i = 1, 2$, correspondingly. The numbers in the square brackets shown at each of the contours K and K' in Fig. 5 indicate the sheet numbers on the corresponding Riemann surfaces for $Q_i^{1/2}, i = 1, 2$, on which the contours (or their parts) have to lie with the first number corresponding to $Q_1^{1/2}$.

The formula (3.12) is identical with that obtained by Streszewski and Jędrzejek [5] for their case (b). Again, the proper behaviour of the integrand in (3.12) at the segments (a_1, a_2) and (b_1, b_2) has fixed the formula unambiguously.

Our further investigations of other matrix elements will be simplify greatly by noticing that the formula (3.12) can be obtained also by putting $x_1 = x_2 = B$ in (3.11) (i.e. by putting zero the relevant integrals in (3.11)) and then substituting the JWKB factors into the remaining integrals. Formally, such a procedure is not allowed since the points lying in some vicinity of B are, for sure, not the JWKB points of the fundamental solutions $\psi_{k,L}$ and $\psi_{k,R}, k = 1, 2$. Nevertheless, the final result in (3.12) is such as if they were.

3.3. Non-overlapping classical regions

The matrix element (3.1) for the case shown in Fig. 6 (the case (a) of Streszewski and Jędrzejek [5]) can now be readily written down as follows:

$$\begin{aligned}
 M_{12}^{\text{JWKB}} = & iC_{1,L}C_{2,L}\{i \int_{-\infty}^{A_L} \exp[-i(w_1 + w_2)] \\
 & + i \int_B^C \exp[-i(\tilde{w}_1 + w_2)] + \int_{A_R}^{+\infty} \exp[-i(\tilde{w}_1 + \tilde{w}_2)] + \int_{K_1'} \exp[+i(\tilde{w}_1 - w_2)] \\
 & + \int_{K_2'} \exp[-i(\tilde{w}_1 - \tilde{w}_2)]\} (Q_1 Q_2)^{-1/4} M_{\text{mod}} dx,
 \end{aligned} \quad (3.13)$$

with the contours K_1' and K_2' shown in Fig. 5. The functions $\tilde{w}_i(x)$ are branches of $w_i(x)$ with the cuts along $(-\infty, b_i)$ and such that $\tilde{w}_i(x) = w_i(x), i = 1, 2$, for $\text{Im } x > 0$. The points A_L, B, C, A_R have been chosen as in the previous formulae i.e. at the boundaries of the corresponding 'holes' of the ε^{CAN} -reduced Stokes graphs.

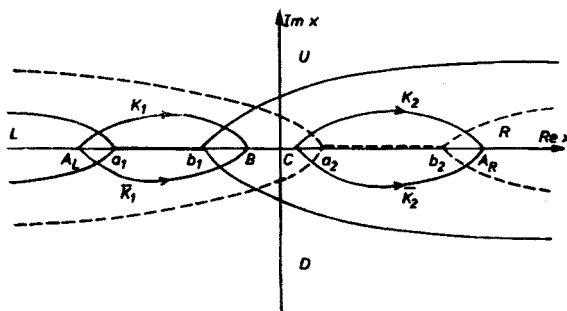


Fig. 6. The Stokes graph corresponding to non-overlapping classical regions of the potentials V_1 and V_2

4. Matrix elements between bound and unbound states

There is nothing special in applying the rules (i)–(iii) of Section 2 to matrix elements between the bound-bound states. The rules can be applied as well to calculate approximately corresponding matrix elements involving also unbound states. The relevant considerations introduce, however, an additional aspect of the matter i.e. an unquantized character of the unbound state energy. This causes, as we shall see, that the relevant integration contours cannot be closed.

To see this let us consider the matrix element (3.1) defined by the potentials sketched in Fig. 7. In comparison with the previous cases we have to consider the fundamental solutions $\psi_{2,U'}$ and $\psi_{2,D'}$ rather than $\psi_{2,R}$ (see Fig. 8). The wave function $\psi_2(x)$ is therefore given by the following chain of equalities:

$$\begin{aligned}\psi_2(x) &= \psi_{2,L'}(x) = \alpha_{2,L'}\psi_{2,U'}(x) + \bar{\alpha}_{2,L'}\psi_{2,D'}(x) \\ &= (\alpha_{2,L'}\beta_{2,U'} + \bar{\alpha}_{2,L'}\bar{\gamma}_{2,U'})\psi_{2,U'}(x) \\ &\quad + (\bar{\alpha}_{2,L'}\bar{\beta}_{2,U'} + \alpha_{2,L'}\gamma_{2,U'})\psi_{2,D'}(x),\end{aligned}\tag{4.1}$$

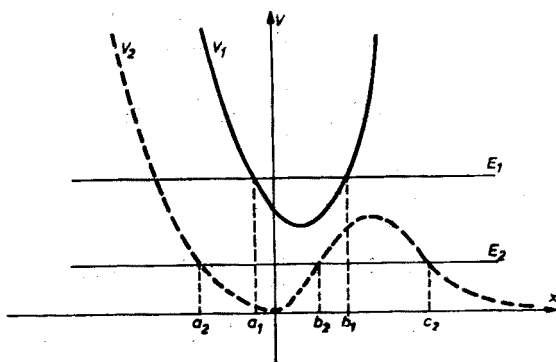


Fig. 7. The case of the potential V_2 without bound states

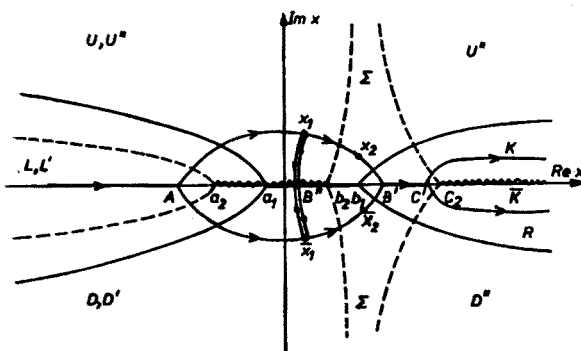


Fig. 8. The Stokes graph corresponding to Fig. 7

where $\alpha_{2,L'} (\equiv \alpha_{2,L'/U' \rightarrow D'})$, $\beta_{2,U'} (\equiv \alpha_{2,U'/U'' \rightarrow D''})$ and $\gamma_{2,U'} (\equiv \alpha_{2,U'/D'' \rightarrow U''})$ can be found with the help of the formulae (A1.16). The x -plane for the ψ_2 -fundamental solutions is cut as in Fig. 8 and the solutions $\psi_{2,U''}$ and $\psi_{2,D''}$ are:

$$\psi_{2,U''}(x) = Q_2^{-1/4} \exp[-iu_2(x)] \chi_{2,U''}(x), \quad x \in U''$$

and

$$\psi_{2,D''}(x) = \bar{\psi}_{2,U''}(\bar{x}), \quad x \in D'' \quad (4.2)$$

where $u_2(x) = \int_{c_2}^x Q_2^{1/2} dy$ is defined in the x -plane with the relevant cuts along $(-\infty, b_2)$ and $(c_2, +\infty)$. The corresponding representations for the remaining ψ_2 -solutions are given as before by (3.4). The coefficients $\alpha_{2,L'}$, $\beta_{2,U'}$ and $\gamma_{2,U'}$ in (4.1) are given in the JWKB approximation by:

$$\alpha_{2,L'}^{\text{JWKB}} = 1 \quad \text{and} \quad \beta_{2,U'}^{\text{JWKB}} = -\gamma_{2,U'}^{\text{JWKB}} = -i \exp[iw_2(c_2)]. \quad (4.3)$$

Analysing, in a way similar to that in Section 3.1, mutual relations between JWKB approximations to the solutions $\psi_{2,L'}, \dots, \psi_{2,D''}$ one finds that $\psi_{2,U'}^{\text{JWKB}}$ is an $\varepsilon_n^{\text{CAN}}$ -part of $\psi_{2,D'}$ in $V_{2,U'}' = K_{2\varepsilon,L'}^{\text{CAN}(n)} \cap K_{2\varepsilon,U'}^{\text{CAN}(n)} \cap K_{2\varepsilon,D'}^{\text{CAN}(n)} \cap U'$ (with the opposite relation in $V_{2,D'}'$). Similarly, $\psi_{2,U''}^{\text{JWKB}}$ is an $\varepsilon_n^{\text{CAN}}$ -part of $\psi_{2,D''}$ in $V_{2,U''} = U'' \cap K_{2\varepsilon,U''}^{\text{CAN}(n)} \cap K_{2\varepsilon,U'}^{\text{CAN}(n)}$ and vice versa. Also, $\psi_{2,U'}^{\text{JWKB}}$ and $\psi_{2,D'}^{\text{JWKB}}$ are ε -parts of each of the approximations $\psi_{2,U'}^{\text{JWKB}}$ and $\psi_{2,D'}^{\text{JWKB}}$ in $V_{2\varepsilon,\Sigma} = \Sigma \cap K_{2\varepsilon,U'}^{\text{CAN}(n)} \cap K_{2\varepsilon,D'}^{\text{CAN}(n)} \cap K_{2\varepsilon,U''}^{\text{CAN}(n)} \cap K_{2\varepsilon,D''}^{\text{CAN}(n)}$, where Σ is a stripe shown in Fig. 8.

Writing the desired JWKB approximations and giving them elegant contour integration forms we have made use of the possibility of adding to (or neglecting in) the dominant integral formulae the following terms:

a) any $\varepsilon_n^{\text{CAN}}$ -part of these formulae i.e. any subdominant one and

b) any 'overdominating' integral formulae since the JWKB approximation to the latter has to vanish.

We have considered all possible relative positions of the classical turning points relevant to the case. The corresponding results are collected in Table II.

TABLE II

Case	α	β	γ	δ	λ	JWKB approximation
1	a_1	b_1	a_2	b_2	c_2	$I_A + I_{BC} + I_1 + I_4^{P'} + I_6$
2	a_1	a_2	b_1	b_2	c_2	$I_A + I_2^{P'} + I_6$
3	a_2	a_1	b_1	b_2	c_2	$I_A + I_2^{P'} + I_6$
4	a_1	a_2	b_2	b_1	c_2	$I_A + I_2^{P'} + I_5^{P'} + I_6$
5	a_2	a_1	b_2	b_1	c_2	$I_A + I_2^{P'} - I_2^{P',bis} + I_6$
6	a_2	b_2	a_1	b_1	c_2	$I_A + I_{B'C} + I_1 + I_3^P + I_6$
7	a_2	a_1	b_2	c_2	b_1	$I_A + I_9$
8	a_2	b_2	a_1	c_2	b_1	$I_A + I_3^P + I_7$
9	a_2	b_2	c_2	a_1	b_1	$I_A + I_3^P + I_8$

A typical example of the corresponding calculations is provided, for example, by the case 5 of Table II (see Fig. 8). By reasoning as in the case of the overlapping classical regions of Section 3 we obtain:

$$\begin{aligned}
 \int_A^{+\infty} \psi_1 M \psi_2 dx &= C_{1L} \{ \alpha_{2,L} \int_A^{x_1} \psi_{1,L} M \psi_{2,U} dx + \bar{\alpha}_{1,L} \alpha_{2,L} \int_{x_1}^{B''} \psi_{1,D} M \psi_{2,U} dx \\
 &+ \alpha_{1,L} \bar{\alpha}_{2,L} \int_{B''}^{x_1} \psi_{1,U} M \psi_{2,D} dx + \alpha_{1,L} \int_{x_1}^{x_2} \psi_{1,U} M (\beta \psi_{2,U} + \gamma \psi_{2,U''}) dx \\
 &+ \alpha_{1,L} \int_{x_2}^{B'} \psi_{1,U} M (\beta \psi_{2,U} + \gamma \psi_{2,U''}) dx + \text{c.c.} \} \\
 &+ \{ C_{1,R} \beta' \int_K \psi_{1,R} M \psi_{2,U''} dx + \text{c.c.} \} \\
 &+ C_{1,R} \int_{B'}^{C'} \psi_{1,R} M (\beta \psi_{2,U} + \gamma \psi_{2,U''}) dx, \quad (4.4)
 \end{aligned}$$

where c.c. means complex conjugation of the predecessors in (4.4) i.e. the corresponding integrations below the real axis and where $\beta = \alpha_{2,L} + \bar{\alpha}_{2,L} \alpha_{2,D'/U' \rightarrow U''}$, $\gamma = \bar{\alpha}_{2,L} \alpha_{2,D'/U'' \rightarrow U'}$ and $\beta' = \alpha_{2,L} \beta_{2,U'} + \bar{\alpha}_{2,L} \bar{\gamma}_{2,U'}$. These coefficients have the following JWKB forms:

$$\beta^{\text{JWKB}} = 1 + \exp [i w_2^-(b_2) - i w_2^+(b_2)],$$

and

$$\gamma^{\text{JWKB}} = i \exp [-i w_2^+(c_2)], \quad \beta'^{\text{JWKB}} = -i \{ \exp [i w_2^-(c_2)] + \exp [i w_2^+(c_2)] \}. \quad (4.5)$$

The point x_1 in (4.4) lies in $U' \cap K_{2e,D'}^{\text{CAN}(n)} \cap K_{2e,U'}^{\text{CAN}(n)} \cap K_{2e,U''}^{\text{CAN}(n)}$ and x_2 — in $K_{2e,U'}^{\text{CAN}(n)} \cap K_{2e,U''}^{\text{CAN}(n)} \cap \Sigma$. Let us note that we could neglect the second term in the fifth integral in (4.4) but we cannot do it in the integrations between x_1 and x_2 since both the integrated terms are comparable in this region. Therefore, we shall also keep up the last term in (4.4) continuing in this way the integration contour between x_1 and x_2 up to the point B' .

For an analogous reason we shall also add to (4.4) a term $C_{1,L} \alpha_{1,L} \beta \int_{B''}^{x_1} \psi_{1,U} M \psi_{2,U} dx$ (+ c.c.) which is *subdominant* in comparison with the third integral in (4.4). Similarly, we shall add the term $C_{1,L} \beta^{\text{JWKB}} \int_A^{B''} \psi_{1,L} M_{\text{mod}}^{\text{JWKB}} \psi_{2,L}^{\text{JWKB}} dx$ (+ c.c.) which should vanish as being '*overdominating*' in comparison with the proper JWKB approximation to the integral $C_{1,L} \beta \int_A^{B''} \psi_{1,L} M \psi_{2,L} dx$.

Collecting all these terms and replacing each fundamental solution in (4.3) as well as each coefficient present there by their JWKB approximations we shall arrive at the formula given in Table II. The remaining formulae in this table can be obtained in a similar way.

The integrals appearing in Table II have the following forms:

$$\begin{aligned}
 I_A &= - \int_{-\infty}^A G_{12}^- dx, \\
 I_{BC} &= - \int_B^C G_{12}^- dx, \\
 I_{B'C'} &= 2 \cos w_2(b_2) \exp[-iw_2^+(b_2)] \int_{B'}^{C'} F_{12}^- dx, \\
 I &= 2 \cos w_2(b_2) \exp[-iw_2^+(b_2)] \int_K G_{12}^+ dx, \\
 I_1 &= i \int_{K_1} F_{12}^+ dx, \quad I_{2,\pm}^{P'} = i \int_{K_2^{P'}} F_{12}^\pm dx, \\
 I_{2,\text{bis}}^{P'} &= 2i \cos w_2(b_2) \exp[-iw_2^+(b_2)] \int_{K_2^{P'}} G_{12}^- dx, \\
 I_3^P &= i \int_{K_3^P} F_{12}^- dx, \quad I_4^{P'} = \int_{K_4^{P'}} F_{12}^- dx, \quad I_5^{P'} = i \int_{K_5^{P'}} F_{12}^+ dx, \\
 I_6 &= 2 \cos w_2(b_2) \exp[+iu_2(b_2)] \int_{K_6} G_{12}^- dx, \\
 I_7 &= 2i \cos w_2(b_2) \exp[-iw_2^+(b_2)] \int_{K_7} G_{12}^+ dx, \\
 I_8 &= 2i \cos w_2(b_2) \exp[-iw_2^+(b_2)] \int_{K_8} G_{12}^- dx, \\
 I_9 &= i \int_{K_2^{P'} + K_9} \{F_{12}^- + 2 \cos w_2(b_2) \exp[-iw_2(b_2)] G_{12}^-\} dx,
 \end{aligned}$$

where

$$F_{12}^\pm(x) = C_{1,L}(Q_1 Q_2)^{-1/4} M_{\text{mod}} \exp[\pm i(w_1 - w_2)],$$

and

$$G_{1,2}^\pm(x) = C_{1,L}(Q_1 Q_2)^{-1/4} M_{\text{mod}} \exp[\pm i(w_1 + w_2)], \quad (4.7)$$

and $F_{12}^\pm(x)$, ..., $G_{12}^\pm(x)$ can be obtained from (4.7) by suitable substitutions $w_i(x)$ by $\tilde{w}_i(x)$, $i = 1, 2$.

All the contours in (4.6) are shown in Fig. 9 where the Riemann surface of the function $(Q_1 Q_2)^{-1/4}$ is sketched. The way of constructing it is completely analogous to that of Fig. 5. Since the forms of the contours in the Riemann surfaces of the functions $Q_i^{1/2}$, $i = 1, 2$, are the same we have collected the numbers of the sheets corresponding to each contour in Table III (in square brackets) with the first number corresponding to the $Q_1^{1/2}$ — Riemann surface. The numbers ± 1 and $\pm i$ also shown in Fig. 9 and attached to the arrows pointed to the corresponding edges of the cuts should multiply the function $(Q_1 Q_2)^{-1/4}$ in

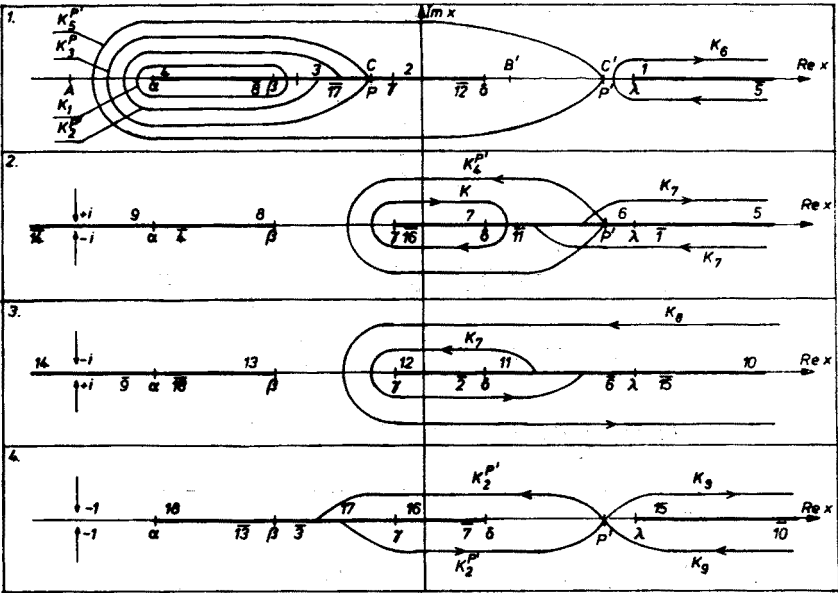


Fig. 9. The Riemann surface for $(Q_1Q_2)^{-1/4}$ with the integration contours corresponding to the potentials shown in Fig. 7

TABLE III

Sheet number of $(Q_1Q_2)^{-1/4}$	Contours	Sheet number of	
		$Q_1^{1/2}$	$Q_2^{1/2}$
1	$K_1, K_2^P, K_3^P, K_5^P, K_6$	1	1
2	K	2	1
	$K_4^{P'}, K_7$	1	2
3	K_7	2	1
4	$K_2^{P'}$	2	2
	K_9	1	1

the integral formulae (4.6) if one wants to perform all the integrations in the first sheet of the figure. Of course, the signs of the functions $w_i(x)$, $i = 1, 2$, in the exponentials in (4.7) should then be also suitably changed according to Table III.

Two comments about the contours with the superscripts P and P' are in order here. First, these contours are not closed: they start and terminate at the corresponding points P and P' but the corresponding integrands do not return to their initial values in these points. Of course, such a behaviour of these integrands is related directly to an unquantized character of the energy E_2 . It causes that the total change of the function $w_2(x)$ going once round the cut (a_2, b_2) is then rather arbitrary than equal to $(2n+1)\pi i$. Secondly, the points P and P' (as well as the points A, B, C and B', C') are not chosen arbitrarily. They are fixed

and have to lie at the boundaries of suitable 'holes' of the corresponding $\varepsilon_n^{\text{CAN}}$ — reduced Stokes graphs $S_{1,e}''$ and $S_{2,e}''$ (see Fig. 15).

On the other hand, the remaining contours are closed (some of them at $+\infty$).

5. Matrix element approximated with the generalized JWKB formulae

The examples considered in Sections 3 and 4 should be convincing enough in showing that the rules (i)–(iii) of Section 2 allow to obtain explicitly the JWKB approximations for each particular matrix element as well as to demonstrate some technicalities of the corresponding procedures. Therefore, the present Section is devoted only to a discussion of some complications arising when the generalized JWKB formulae [6] are used to approximate the integrated wave functions.

In spite of the apparent complications arising in such a case the rules (i)–(iii) as well as the corresponding integration procedures remain unchanged. Consider, for example, the matrix element (3.1) defined by Fig. 3. In order not to complicate excessively our further considerations we limit ourselves to the case of the 1th generalized JWKB formulae with the corresponding Stokes graphs shown in Fig. 10. Only the system of the cuts for the function $(Q_1 Q_2)^{-1/4}$ can affect the formulae (3.12). However, it causes merely the integration contour K' in (3.12) to run in a way shown in Fig. 11 where the Riemann surface corresponding to Fig. 10 is drawn. The subsequent parts of the integration contour are numbered in Fig. 11 by the Roman figures.

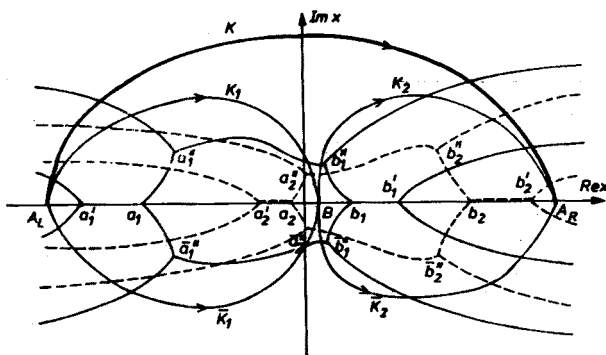


Fig. 10. The Stokes graph corresponding to Fig. 3 with the 1th generalized JWKB formulae used as approximations

6. Limitations to the rules

Applications of the rules (i)–(iii) in Section 2 can fail, in general, when the corresponding integration contours cannot be drawn according to the prescriptions provided by the rules. First of all this can happen if Stokes graphs corresponding to considered cases are not the JWKB approximation allowing graphs (see Appendix 1). An example of such Stokes graphs is considered below. They appear most likely for lowest energy levels

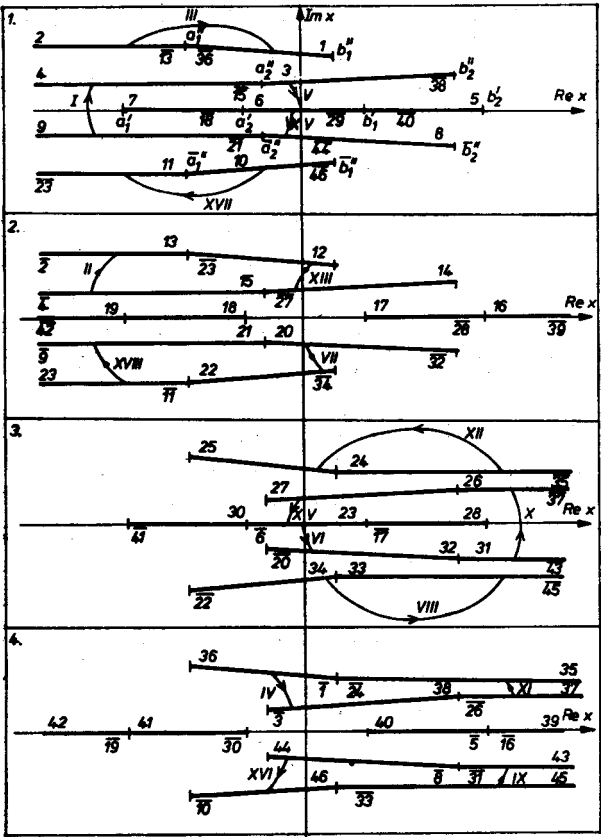


Fig. 11. The Riemann surface for $(Q_1 Q_2)^{-1/4}$ with the integration contour corresponding to the case shown in Fig. 10

but also for these levels which lie closely to the bottom of some potential well but below it. In such cases the relevant ‘holes’ of the ε -reduced Stokes graphs overlap making impossible the canonical communication of some of the relevant ε -reduced sectors. A consequence of this are false results of the analytical continuations of the corresponding JWKB approximations and, therefore, an application of the rule (i) must lead us to wrong results also.

However, there are also matrix elements where the rules cannot be applied successfully even if the Stokes graphs corresponding to such cases are the JWKB approximation allowing graphs. A simple situation of this kind is provided by the case of non-orthogonal matrix elements with the overlapping classical regions considered in Section 3.2. If the classical turning points a_1 and b_2 are too close to each other then the ‘holes’ corresponding to them and lying in the different ε -reduced Stokes graphs $S_{1,\varepsilon}$ and $S_{2,\varepsilon}$ can overlap (see Fig. 12). Consequently, the formula (3.12) cannot give a good approximation to the integral considered in this case. However, it can be modified. The price paid for this is to resign from satisfying the rule (iii). Consequently, the property of the approximate formulae to be unique is now lost.

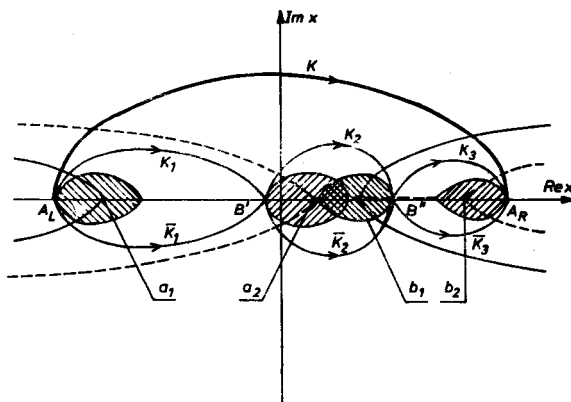


Fig. 12. The Stokes graph and integration contours in the case when some of the rules (i)–(iii) of Section 2 cannot be applied

The integration can be performed in this case according to Fig. 12 leading us to the following approximate formula:

$$\int_{A_L}^{A_R} [\psi_1 M \psi_2]^{JWKB} dx = i C_{1,L} C_{2,L} \left\{ \int_{K_1'} \exp [+i(w_1 - w_2)] + \int_{K_2'} \cos(w_1 - w_2) + \int_{K_3'} \exp [-i(w_1 - w_2)] \right\} (Q_1 Q_2)^{-1/4} M_{\text{mod}} dx. \quad (6.1)$$

Of course, the integration contours $K_i' = K_i - \bar{K}_i$, $i = 1, 2, 3$, cannot be closed in (6.1).

There are yet possible formulae other than this given above. They cannot be excluded with the rules (i) and (ii) only. The choice made above is, therefore, arbitrary. The proper choice can be done in such cases only with the aid of the numerical tests.

As we have already mentioned there are matrix elements for which none of the above procedure is possible. A corresponding example is provided by the broken supersymmetric quantum mechanics (SUSY QM) [7, 10–12] if matrix elements between the ground-state and any other eigen state of the underlying theory are considered.

In its simplest version the potential of the broken SUSY QM is given by $V(x) = (1/2)[U'(x)]^2 - (1/2)\hbar U''(x)$ where superpotential $U(x) = x(x^2 - \alpha^2)$. The potential $V(x)$ has then a form shown in Fig. 13. It is known from the theory of the broken SUSY QM that the ground-state energy level E_0 lies between zero and the higher local minimum of $V(x)$ (see Fig. 13) and its value is exponentially small in \hbar (if $\hbar \ll U(x_+) - U(x_-)$ [7]). The Stokes' graph corresponding to the level looks like in Fig. 14. The remaining energy levels all lie above the higher minimum in Fig. 13.

Consider the following matrix element:

$$\int_A^B \psi_{E_0} M \psi_E dx, \quad (6.2)$$

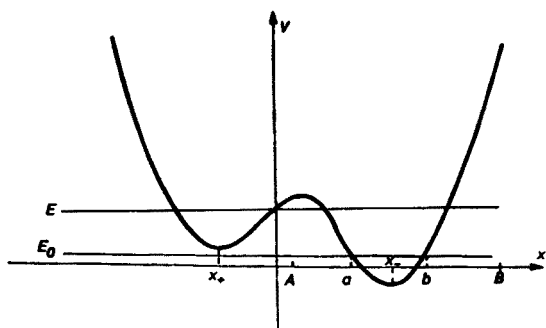


Fig. 13. A typical potential of supersymmetric quantum mechanics

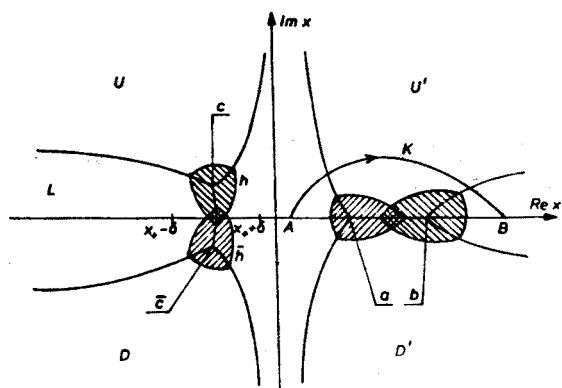


Fig. 14. The Stokes graph corresponding to Fig. 13 with the indicated 'holes'

with $E > E_0$ (see Fig. 13). The experience gained from the previous examples suggests to deform the integration contour from the real axis to the contour K and next to make use of the fundamental solutions $\psi_{E_0,X}(x)$ and $\psi_{E,X}(x)$, $X = L, U', D', R$, (corresponding to the Stokes' graph in Fig. 14) in the way similar to that leading to the formula (3.10). It demands, however, to express the fundamental solutions $\psi_{X,L}$ and $\psi_{X,R}$ by the fundamental solutions $\psi_{X,Y}$, $X = E_0, E$, $Y = U', D'$. There is nothing particular in such a procedure when the solutions $\psi_{E,Y}$, $Y = L, U', D', R$, are considered (with $E > E_0$). However, considering the solutions $\psi_{E_0,Y}$, $Y = L, \dots, R$, we have to calculate quantities such as $\chi_{E_0,L \rightarrow U'}$ or $\chi_{E_0,U' \rightarrow D'}$ (see Appendix 1). Approximating next (6.2) by the JWKB formulae we would like to put: $\chi_{E_0,L \rightarrow U'}^{\text{JWKB}} = \chi_{E_0,U' \rightarrow D'}^{\text{JWKB}} = 1$. However, it would be wrong. These quantities cannot be approximated in this way. The reason is that the pairs c, \bar{c} and a, b of the singular points lie too close to each other ($c \sim x_+ + i\delta$, $\bar{c} \sim x_+ - i\delta$, $a \sim x_- - i\delta$, $b \sim x_- + i\delta$, where $\delta^2 = \hbar/(2\sqrt{3}\alpha)$, if $\hbar \ll 2\sqrt{3}\alpha^3 \sim U(x_+) - U(x_-)$; see Giler et al. [7]). Therefore, the pairs of the singularities at c, \bar{c} and a, b contribute substantially to $\chi_{E_0,L \rightarrow U'}$ and $\chi_{E_0,U' \rightarrow D'}$ correspondingly, strongly deviating the values of these quantities from unity (see Appendix 3 for simple estimations). Speaking in other words it means that the canonical index of the Stokes graph in Fig. 14 has to be greater than unity.

One can check, on the other hand, that there is no way of expressing (6.2) in terms of the solutions $\psi_{E_0, Y}$, $Y = U, D, U', D'$, eliminating simultaneously both the quantities $\chi_{E_0, L \rightarrow U'}$ and $\chi_{E_0, U' \rightarrow D'}$ from the corresponding considerations.

It follows, therefore, that in the considered case one cannot perform a good JWKB approximations in (6.2) since the relevant integration contours have to pass the regions of overlapping 'holes' h and \bar{h} of the ε -reduced Stokes graph corresponding to the graph in Fig. 14.

Let us note, however, that the corresponding quantization condition for the energy E_0 can be written in such a way that both the troublesome quantities $\chi_{E_0, L \rightarrow U'}$ and $\chi_{E_0, U' \rightarrow D'}$ can be get rid of it. A different matter is that making the usual JWKB approximations in the quantization condition we would obtain a result being in accordance with the assumed accuracy of the method (i.e. zero) but too crude in comparison with the actual value of the level [7].

6. Summary: comments and conclusions

In this paper we have formulated the rules for the matrix element calculations in the JWKB approximation (with the extended meaning of the latter — see footnote in Section 1).

The necessary and sufficient conditions relevant for applications of the rules have been formulated in Appendix 1. The conditions have been based on the properties of the canonical indices of the Stokes graphs.

The canonical indices being global characteristics for the Stokes graphs have appeared to be extremely useful as suitable quantitative estimators of the JWKB approximations.

The examples of matrix elements we have considered in the paper illustrate the following general procedure which has to be applied if the results obtained with the rules are to be under a control:

1. check that canonical indices (up to a desired order) of the considered Stokes graphs are sufficiently small in comparison with unity;
2. apply the rules (i)–(iii) of Section 2;
3. if the considered matrix elements are the non-orthogonal ones check additionally whether the property of Section 3 is fulfilled.

The following comment about the canonical indices seems to be in order here. We have found the 0th canonical index for the harmonic oscillator. In general, however, the indices can be difficult to find. On the other hand it seems that even the values of the integrals $\int_{\infty D_1}^{\infty D_2} |\omega Q^{1/2} dx|$ calculated along some suitably chosen canonical paths which do not necessarily extremize the integrals can provide a good portion of information about possibilities of applying the relevant JWKB approximations.

Another comment is related to the final integration contours. As it has been shown in Section 4 we can make use of both the subdominant behaviour and the 'overdominant' one of some integrals in order to give the approximated matrix elements compact and elegant forms of contour integrations. However, the closed contours appear rather rarely

and, in fact, only when they round the classically allowed region of the quantized potential well. Therefore, for matrix elements with both energies unquantized (but with finite limits of integrations) none of the integration contours will be closed.

If the tests suggested by the points 1–3 above fail for some of the points one has to proceed in different ways. One can apply as in Section 6 only some of the rules expecting, therefore, the worse results as the price of this.

However, it can happen that one can also obtain good results applying *all* the rules even if such disadvantageous situations take place. This can happen, for example, if the integration contours run through the regions containing only turning points with well canonical separations. In such cases the relevant accuracy is determined rather by less global quantities such as canonical indices of the canonical paths. Therefore, a detailed examination of such seemingly untractable cases can reveal possibilities for applying the JWKB approximation with a good and controlled accuracy.

Finally, it should be stressed that the conditions for the JWKB approximation to be applied formulated in Appendix 1 are valid also when *any* quantum-mechanical quantity are to be calculated in this approximation.

I would like to thank dr P. Kosiński for many valuable discussions as well as for careful reading of the manuscript.

APPENDIX 1

We summarize here the main ideas and properties of the Stokes graph and of the fundamental set of solutions it defines. We also introduce in this Appendix the notions of the JWKB points of the fundamental solutions, their canonical points as well as several other important notions which are widely used throughout the paper. The lack of the satisfactory references we could refered to is the reason for such extended discussion of the underlying notions as given below.

A1.1. Fundamental solutions to the Schroedinger equation

Consider the Schroedinger equation:

$$\psi''(x) - q(x)\psi(x) = 0, \quad (\text{A1.1})$$

where $q(x) = 2m(V(x) - E)/\hbar^2$. It has been noticed by Fröman and Fröman [3] that the following substitutions:

$$\psi(x) = Q^{-1/4}(x)\varphi(x) \quad (\text{A1.2})$$

and:

$$\xi(x_0, x) = \int_{x_0}^x Q^{1/2}(y)dy, \quad (\text{A1.3})$$

with $\varphi(x)$ as the new wave function and with ξ as the new independent variable in (A1.1), do not change the form of the Schroedinger equation i.e. for $\tilde{\varphi}(\xi(x)) \equiv \varphi(x)$ we have the following equation:

$$\tilde{\varphi}(\xi) - (1 + \tilde{\omega}(\xi))\tilde{\varphi}(x) = 0, \quad (\text{A1.4})$$

with

$$\tilde{w}(\xi) = (\hat{q} - \tilde{Q})/\tilde{q} + \tilde{Q}^{-1/4}(d^2/d\xi^2)\tilde{Q}^{1/4} \quad (\text{A1.5})$$

or

$$\omega(x) = (q - Q)/q + Q^{-3/4}(d^2/dx^2)Q^{-1/4}, \quad (\text{A1.6})$$

where $\tilde{f}(\xi(x)) \equiv f(x)$, $f = q, Q, \omega$.

The function $Q(x)$ in (A1.2) and (A1.3) can be an arbitrary function of the complex variable x (holomorphic or singular). However, for simplicity, we consider $Q(x)$ (as well as $q(x)$) to be a meromorphic function but holomorphic in the neighbourhood of the real axis.

The zeros of $q(x)$ and $Q(x)$ are singular points for the function $\omega(x)$. They are called turning points and generalized turning points respectively. The real turning points are called classical turning points.

Let $\{x_i: Q(x_i) = 0\}$ be the set of zeros of $Q(x)$. The lines $\text{Re} \int_{x_i}^x Q^{1/2} dy = 0$ (for each x_i) are called the Stokes lines. A set of all the Stokes lines is called a Stokes graph.

Let a domain $D = \{x: \sigma \text{Re} \int_{x_i}^x Q^{1/2} dy < 0\}$ do not contain any Stokes line for some x_i and $\sigma = \pm 1$. Such a domain will be called a sector. For each sector D the following solution of the equation (A1.4) can be constructed [3, 13]:

$$\varphi_D(x) = \exp \left[+\sigma \int_{x_i}^x Q^{1/2} dy \right] \chi_D(x), \quad (\text{A1.7})$$

where

$$\begin{aligned} \chi_D(x) &= 1 + \frac{\sigma}{2} \int_{\gamma_D(x)} \omega Q^{1/2} \{1 - \exp [2\sigma \xi(x, y)]\} \chi_D dy \\ &= 1 + \sum_{n \geq 1} \left(\frac{\sigma}{2} \right)^n \int_{\gamma_D(x)} dy_1 \int_{\gamma_D(y_1)} dy_2 \dots \int_{\gamma_D(y_{n-1})} dy_n \omega(y_1) \omega(y_2) \dots \omega(y_n) \\ &\quad \times (Q_1 Q_2 \dots Q_n)^{1/2} \{1 - \exp [2\sigma \xi(x, y_1)]\} \\ &\quad \times \{1 - \exp [2\sigma \xi(y_1, y_2)]\} \dots \{1 - \exp [2\sigma \xi(y_{n-1}, y_n)]\} \end{aligned} \quad (\text{A1.8})$$

and $\gamma_D(x)$ is a path starting from the infinity ∞_D of the sector D and ending at the point x , for which the following inequality is fulfilled:

$$\frac{1}{2} C_{\gamma_D}(x) \int_{\gamma_D(x)} |\omega(y) Q^{1/2}(y) dy| < +\infty, \quad (\text{A1.9})$$

with

$$C_{\gamma_D}(x) = \max_{y, z \in \gamma_D(x)} |1 - \exp [2\sigma \xi(y, z)]|, \quad (\text{A1.10})$$

where the points y, z are ordered on $\gamma_D(x)$ i.e. y lies on the path $\gamma_D(x)$ between x and z . For any such a path the function $\gamma_D(x)$ fulfils the following bound:

$$|\chi_D(x) - 1| \leq \exp [\varrho_D(x)] - 1 \quad (\text{A1.11})$$

where

$$\varrho_D(x) = \liminf \left[\frac{1}{2} C_{\gamma_D}(x) \int_{\gamma_D(x)} |\omega(y) Q^{1/2} dy| \right] \quad (\text{A1.12})$$

and the limit in (A1.12) is taken for all γ_D 's fulfilling (A1.9).

Let K_D denote a set of all the points x fulfilling (A1.9) for some path $\gamma_D(x)$. It follows from (A1.11) that the series in (A1.8) is uniformly convergent in K_D .

The solution $\psi_D(x)$ to the Schroedinger equation (A1.1) defined by (A1.2), (A1.7) and (A1.8) can, therefore, be written in the form:

$$\psi_D(x) = \psi_D^{\text{JWKB}}(x) \chi_D(x), \quad (\text{A1.13})$$

with

$$\psi_D^{\text{JWKB}}(x) = Q^{-1/4} \exp \left[+ \sigma \int_{x_i}^x Q^{1/2} dy \right] \quad (\text{A1.14})$$

and $\chi_D(x)$ given by (A1.8).

The solution $\psi_D(x)$ vanishing at ∞_D and having this property is unique in D (up to a multiplicative constant).

Each particular Stokes graph defines its own set of the solutions to the Schroedinger equation having the form (A1.13). We shall call such a set a fundamental set and each solution it contains — a fundamental solution.

The fundamental solution $\psi_D(x)$ defined in the sector D can be continued analytically to any point of the Stokes graph which is regular for $\omega(x)$, preserving its form (A1.13). It increases infinitely when continuing to any other sector of the graph if $x \rightarrow \infty$ in this sector.

Let us note further that any two fundamental solutions defined in different sectors of the Stokes graph are linearly independent. This fact is the obvious consequence of their asymptotic behaviour described above.

On the other hand, any of the fundamental solutions can be expressed as a linear combination of another two fundamental solutions. The coefficients of such a linear combination can be calculated directly by analytic continuation of the solutions to the corresponding sectors of the Stokes graph keeping their form (A1.13). Writing:

$$\psi_i(x) = \alpha_{i/j \rightarrow k} \psi_j(x) + \alpha_{i/k \rightarrow j} \psi_k(x) \quad (\text{A1.15})$$

we have

$$\alpha_{i/j \rightarrow k} = \lim_{x \rightarrow \infty k} [\psi_i(x) / \psi_j(x)]$$

and

$$\alpha_{i/k \rightarrow j} = \lim_{x \rightarrow \infty_j} [\psi_i(x)/\psi_k(x)] \quad (\text{A1.16})$$

where ∞_k, ∞_j are the infinity points at the sectors D_k, D_j respectively.

It should also be noticed that, due to our assumptions about $q(x)$ and $Q(x)$, the formulae (A1.7) and (A1.8) define the solutions which are meromorphic in the x -plane but are holomorphic in the neighbourhood of the real axis. However, the representations of the solutions given by (A1.7) and (A1.8) are singular at each turning point (whether real or complex).

One can meet the following particular choices of $Q(x)$:

1. $Q(x) = q(x)$
2. $Q(x) = Q_{\text{mod}} \sum_{n=0}^M Y_{2n}(x) \quad (\text{Fröman and Fröman [2, 8]})$
3. $Q(x) = q(x)q_1(x) \dots q_n(x) \quad (\text{Giler [6]}) \quad (\text{A1.17})$

Note also that $Q(x)$ can be suitably chosen for each singular point of $q(x)$ [2, 8].

A1.2. The JWKB approximation to the fundamental solutions

Let us now discuss briefly the properties of the fundamental solutions which are most important for their approximations by the JWKB factors (A1.14). First, as it follows from (A1.8), if $x \rightarrow \infty_D$ then $\chi_D(x) \rightarrow 1$ and therefore in such a limit

$$\psi_D(x) \sim \psi_D^{\text{JWKB}}(x). \quad (\text{A1.18})$$

However, it is seen from (A1.11), (A1.13) and (A1.14) that the approximation (A1.18) can be useful not only asymptotically when $x \rightarrow \infty_D$ but also for finite x , for which the following condition can be satisfied:

$$\varrho_D(x) < \varepsilon \ll 1. \quad (\text{A1.19})$$

Each such a point x will be called a JWKB point of the fundamental solution $\psi_D(x)$.

A set of all the JWKB points for the solution $\psi_D(x)$ fulfilling (A1.19) for a given ε will be denoted by $K_{\varepsilon, D}^{\text{JWKB}}$.

A1.3. Canonical points and canonical domains of the fundamental solutions

The property of the point x to be the JWKB point of the solution $\psi_D(x)$ depends on its position in the x -plane and is strongly related to its another possible property of being a canonical point of the solution $\psi_D(x)$ in the following sense [13]:

A point x is a canonical point of the solution $\psi_D(x)$ if a path $\gamma_D(x)$ exists for which each ordered pair (y, z) of the points y and z lying on the path (with y between x and z) fulfils:

$$\text{Re}[\sigma \xi(y, z)] \leq 0. \quad (\text{A1.20})$$

A path $\gamma_D(x)$ with the property (A1.20) is called a canonical path [13].

It follows from (A1.9) that for the canonical points of $\psi_D(x)$ the coefficient $C_{\gamma_D}(x)$

cannot be greater than 2. Therefore, the condition (A1.19) for the JWKB points can be reduced to:

$$\varrho_D^{\text{CAN}}(x) = \liminf_{\gamma_D^{\text{CAN}}(x)} \int |\omega(y) Q^{1/2} dy| < \varepsilon \ll 1 \quad (\text{A1.21})$$

if these points coincide with the canonical ones.

The canonical points for the solution $\psi_D(x)$ seem to be the most probable candidates also for its JWKB points (for some ε in (A1.21)). On the other hand the condition (A1.19) can hardly be satisfied by the *non*-canonical points for which the coefficient $C_{\gamma_D}(x)$ can be an arbitrary real number (depending on x and $\gamma_D(x)$).

An identification of the canonical points for each particular fundamental solution is a relatively simple task. A set K_D^{CAN} of all canonical points of the solution $\psi_D(x)$ is called a canonical domain of $\psi_D(x)$ [13]. A boundary of the canonical domain K_D^{CAN} consists of the Stokes lines. Some examples of the canonical domains are considered in Section 3.

The sectors D_i and D_j , $i \neq j$, are said to be communicating canonically if $D_i, D_j \subset K_{D_i}^{\text{CAN}} \cap K_{D_j}^{\text{CAN}} \neq \emptyset$.

The following 'canonical' properties of the fundamental solutions are most important for our further considerations.

1. The infinity points of the communicating canonically sectors can be connected by some canonical path.

2. Let D_i , $i = 1, 2, 3$, be the pairwise canonically communicating sectors. It follows then that for the corresponding solutions ψ_{D_i} , $i = 1, 2, 3$, the coefficients $\alpha_{D_i/D_j \rightarrow D_k}$, $\alpha_{D_i/D_k \rightarrow D_j}$, ... etc., $i, j, k = 1, 2, 3$, of the corresponding linear combination (A1.15) can be calculated by (A1.16) keeping x running to the infinities ∞_{D_j} , ∞_{D_k} , ... etc. along the corresponding *canonical* paths $\gamma_{D_i}(\infty_k)$, $\gamma_{D_j}(\infty_k)$, ... etc. Such α -coefficients we shall call canonical coefficients.

3. If D_0 and D_{n+1} are not communicating canonical domains then it is always possible to find a sequence D_1, D_2, \dots, D_n of the sectors such that in each of the triads (D_p, D_{p+1}, D_{p+2}) $p = 0, 1, \dots, n-1$, the sectors communicate canonically pairwise.

4. It follows, therefore, that in each linear relation (A1.15) its coefficients are either the canonical coefficients or can be expressed as functions of such coefficients.

The last two properties justify the following two statements expressing the importance of the fundamental solutions and their canonical domains in applications:

a) *to solve any global one-dimensional quantum-mechanical problem (such as calculations of matrix elements, energy levels, scattering amplitudes etc.) it is sufficient to use the set of the fundamental solutions; and*

b) *the corresponding considerations which lead to the solution of the problem can be performed completely inside the canonical domains that correspond to the fundamental solutions.*

A1.4. Canonical index of a Stokes graph

Let D_i and D_j be a pair of the communicating canonically sectors and let $\varrho_{ij} \equiv \varrho_{D_i}^{\text{CAN}}(\infty_{D_j})$ where $\varrho_{D_i}^{\text{CAN}}(\infty_{D_j})$ is given by (A1.21) for $x = \infty_{D_j}$. Let R be a set of all ϱ_{ij}

calculated for a given Stokes graph. The following quantity shall prove its usefulness for our further considerations:

$$\varepsilon^{\text{CAN}} = \max_{\varrho_{ij} \in R} \varrho_{ij}. \quad (\text{A1.22})$$

We shall call this quantity a canonical index of a given Stokes graph.

Let Γ_{ij} be a set of all canonical paths starting at ∞_{D_i} and running to ∞_{D_j} . All the paths in Γ_{ij} are homotopically equivalent i.e. there are no the turning points neither the poles of $Q(x)$ and $q(x)$ between them. Therefore, Γ_{ij} will denote also an equivalence class of such paths as well as any representative of the class. Since any canonical path $\gamma_{D_i}(\infty_{D_j})$ can be considered as being an oppositely directed canonical path $\gamma_{D_j}(\infty_{D_i})$ (i.e. $\gamma_{D_i}(\infty_{D_j}) = -\gamma_{D_j}(\infty_{D_i})$) then $\Gamma_{ij} = -\Gamma_{ji}$.

Each class Γ_{ij} divides a set T of all turning points of the Stokes graph into two disjoint parts T_{ij} and T'_{ij} . Each pair, t_{ij} , t'_{ij} of the turning points with $t_{ij} \in T_{ij}$ and $t'_{ij} \in T'_{ij}$ will be said to be canonically well separated if $\varrho_{ij}(= \varrho_{ji})$ fulfils the bound (A1.21) i.e.

$$\varrho_{ij} \ll 1. \quad (\text{A1.23})$$

Each ϱ_{ij} will be called a canonical index of the corresponding path Γ_{ij} .

If the condition (A1.23) is satisfied for each member of the set R then the turning points of a given Stokes graph will be said to be canonically well separated. Obviously, the last condition is equivalent to the following one:

$$\varepsilon^{\text{CAN}} \ll 1. \quad (\text{A1.24})$$

A1.5. Conditions for applicability of the JWKB approximations

Taking into account the canonical properties of the fundamental solutions described in the previous point it seems reasonable to limit further considerations of the JWKB points of a given fundamental solutions ψ_D to a subset $K_{\varepsilon,D}$ of $K_{\varepsilon,D}^{\text{JWKB}}$ defined by

$$K_{\varepsilon,D} = K_D^{\text{CAN}} \cap K_{\varepsilon,D}^{\text{JWKB}} \quad (\text{A1.25})$$

i.e. to this JWKB points of ψ_D which are also its canonical points. Each $K_{\varepsilon,D}$ will be called an ε -reduced canonical domain.

Similarly, a set

$$D_{\varepsilon} = D \cap K_{\varepsilon,D} \quad (\text{A1.26})$$

will be called an ε -reduced sector.

A union $S_{\varepsilon} \equiv \bigcup_{r=1}^p \partial D_{\varepsilon,r}$ of the boundaries of all the ε -reduced sectors will be called an ε -reduced Stokes graph (see Fig. 15). It is seen from Fig. 15 that an ε -reduced Stokes graph is obtained from the corresponding Stokes graph by substituting each turning point by an appropriate 'hole'.

Analogously, two ε -reduced sectors $D_{\varepsilon,i}$ and $D_{\varepsilon,j}$, $i \neq j$, will be said to be canonically communicating if $D_{\varepsilon,i}, D_{\varepsilon,j} \subset K_{\varepsilon,i} \cap K_{\varepsilon,j} \neq \emptyset$.

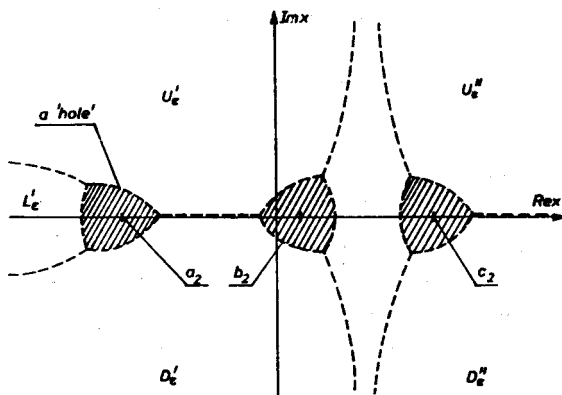


Fig. 15. The ε -reduced Stokes graph corresponding to the Stokes graph of Fig. 8 (drawn with broken lines)

Therefore, to a given Stokes graph S there correspond the sets D_r , ψ_{D_r} and $K_{D_r}^{CAN}$, $r = 1, \dots, p$, of the sectors, the fundamental solutions and their canonical domains respectively, and to the related ε -reduced Stokes graph S_ε there corresponds the sets $D_{\varepsilon,r}$, $\psi_{D_{\varepsilon,r}}^{JWKB}$ and K_{ε,D_r} , $r = 1, \dots, p$, of the ε -reduced sectors, the JWKB approximations to fundamental solutions and their ε -reduced canonical domains. The following statement should now be obvious:

A successful application of the JWKB approximation to solve any (global) one-dimensional quantum mechanical problem requires the canonical properties 1.-4. of the fundamental solutions (stated in the Section A1.3) to remain valid also when the following substitutions is performed: $S \rightarrow S_\varepsilon$, $D_r \rightarrow D_{\varepsilon,r}$, $\psi_{D_r} \rightarrow \psi_{D_{\varepsilon,r}}^{JWKB}$ and $K_{D_r}^{CAN} \rightarrow K_{\varepsilon,D_r}$, $r = 1, \dots, p$, for some $\varepsilon \ll 1$.

If an application of the JWKB approximation such as described in the above statement is possible then the Stokes graph corresponding to the case will be called a JWKB approximation allowing graph.

Let us note further that if a given Stokes graph is the JWKB approximation allowing graph for some $\varepsilon \ll 1$ then ε is in fact fixed and equal to the canonical index of the graph.

This last conclusion follows from an observation that by lowering ε in (A1.21) we shall obtain such a value for which the canonical communication between some of the canonical domains is broken. This can happen, of course, if ε becomes smaller than the canonical index of the considered Stokes graph.

The following condition is, therefore, necessary and sufficient for the Stokes graph S to be the JWKB approximation allowing graph:

The turning points of the Stokes graph S are canonically well separated.

Therefore, the canonical index of the Stokes graph S becomes its basic characteristic which allows to decide whether it is possible or not to make the JWKB approximations to the fundamental solutions globally i.e. in the whole area of the corresponding ε -reduced Stokes graph S_ε .

It follows further that when considering a class of the JWKB approximation allowing graphs we should put everywhere $\varepsilon = \varepsilon^{\text{CAN}}$.

In this way, the canonical index becomes also a basic unit for measuring relevant accuracies with which the JWKB approximations are used in corresponding calculations.

However, the following comment is in order here. It can happen, of course, that a given Stokes' graph is not the JWKB approximation allowing graph. It does not mean, however, that none of the JWKB approximations is then possible to solve any underlying quantum mechanical problem. It means merely that only some particular problems (such as, for example, the energy eigenvalue problem) can be solved in such a case using the JWKB approximations. These are problems which require for their solution only some subsets of the fundamental set and for each such a subset the considered Stokes graph behaves as a JWKB approximation allowing graph.

A1.6. Derivatives of the fundamental solutions and their JWKB approximations

The considerations in Section A1.5 need only slight changes if derivatives of the fundamental solutions are also to be taken into account. One can proceed in the following way.

Let $\psi_D^{(n)}(x)$ be the n th derivative of the fundamental solution $\psi_D(x)$. Writing:

$$\psi_D^{(n)}(x) = \psi_D^{\text{JWKB}}(x) \chi_{D,n}(x) \quad (\text{A1.27})$$

and

$$(\psi_D^{\text{JWKB}}(x))^{(n)} = \alpha_n(x) \psi_D^{\text{JWKB}}(x) \quad (\text{A1.28})$$

we get for $\chi_{D,n}(x)$:

$$\chi_{D,n}(x) = \sum_{k=0}^n \binom{n}{k} \chi_D^{(k)}(x) \alpha_{n-k}(x), \quad (\text{A1.29})$$

where $\chi_D(x)$ is given by (A1.8). It follows from (A1.8) that the k th derivative of $\chi_D(x)$ can be written as:

$$\chi_D^{(k)}(x) = a_k + b_k \chi_D(x) + \sigma d_k \int_{\gamma_D(x)} \omega Q^{1/2} \chi_D dy, \quad (\text{A1.30})$$

where the coefficients α_k , a_k , b_k and d_k are functions of q and Q and their derivatives (more detailed forms of these coefficients will be given below). Therefore, $\chi_{D,n}$ can be given the following form:

$$\chi_{D,n}(x) = A_k(x) + B_k(x) \chi_D(x) + \sigma D_k(x) \int_{\gamma_D(x)} \omega Q^{1/2} \chi_D dy, \quad (\text{A1.31})$$

with

$$A_n(x) = \sum_{k=0}^n \binom{n}{k} a_k(x) \alpha_{n-k}(x) \quad (\text{A1.32})$$

and with similar expressions for B_n and D_n built with b_k and d_k respectively.

Using now the properties of the solutions (A1.8) one can obtain the following bound for $\chi_{D,n}(x)$:

$$|\chi_{D,n}(x) - C_n(x)| \leq (|B_n(x)| + |D_n(x)|) (\exp [\varrho_D(x)] - 1). \tag{A1.33}$$

where $C_n(x) = A_n(x) + B_n(x)$ and $\varrho_D(x)$ is defined by (A1.12). The bound (A1.33) is, of course, a generalization of (A1.11).

It is now natural to limit our further considerations to the ε^{CAN} -reduced canonical domains $K_{\varepsilon,D}^{\text{CAN}}$. It should be obvious that the functions $B_n(x)$, $C_n(x)$ and $D_n(x)$ are holomorphic in $K_{\varepsilon,D}^{\text{CAN}}$. Let $\{x_i: C_n(x_i) = 0, x_i \in K_{\varepsilon,D}^{\text{CAN}}\}$ be a set of zeros of $C_n(x)$ which lie inside $K_{\varepsilon,D}^{\text{CAN}}$ and let V_i be some finite vicinity of x_i . It can be shown, under the assumptions we have made about the functions Q and q , that the function:

$$M_n(x) = (|B_n(x)| + |D_n(x)|)/|C_n(x)| \tag{A1.34}$$

is bounded in $K_{\varepsilon,D}^{\text{CAN}} \setminus \cup V_i$ ($\cup V_i$ is a union of all V_i). Let $M_{n,D}$ be this bound. Obviously, the sum $N_n(x) = |B_n(x)| + |D_n(x)|$ is also bounded in $\cup V_i$ with a bound $N_{n,D}$. The vicinities V_i are assumed to be chosen in a way ensuring a minimalization of $M_{n,D}$ and $N_{n,D}$. Therefore, the function $C_n(x)$ can be a good approximation to $\chi_{D,n}(x)$ for $x \in K_{\varepsilon,D}^{\text{CAN}}$ if the following bound is satisfied:

$$\varepsilon_{n,D}^{\text{CAN}} \ll 1, \tag{A1.35}$$

where $\varepsilon_{n,D}^{\text{CAN}}$ is maximal of the numbers ε^{CAN} , $M_{n,D}\varepsilon^{\text{CAN}}$, $N_{n,D}\varepsilon^{\text{CAN}}$.

A number $\varepsilon_n^{\text{CAN}}$, being maximal of the numbers $\varepsilon_{k,D_i}^{\text{CAN}}$, $i = 1, \dots, p$, $k = 0, 1, \dots, n$, will be called an n th canonical index of a given Stokes graph. Of course, $\varepsilon_0^{\text{CAN}} = \varepsilon^{\text{CAN}}$.

Let $K_{\varepsilon,D}^{\text{CAN}(n)}$ be a set obtained from $K_{\varepsilon,D}^{\text{CAN}}$ by the substitution $\varepsilon^{\text{CAN}} \rightarrow \varepsilon_n^{\text{CAN}}$. It follows then from the above considerations that we get the following formula for the JWKB approximation to $\psi_D^{(k)}(x)$ in $K_{\varepsilon,D}^{\text{CAN}(n)}$:

$$\psi_D^{(k),\text{JWKB}}(x) = C_k(x)\psi_D^{\text{JWKB}}(x), \quad \text{for} \quad \varepsilon_k^{\text{CAN}} \ll 1 \quad k = 0, 1, \dots, n. \tag{A1.36}$$

One can now perform constructions analogous to those of Section A1.5 i.e. the constructions of $\varepsilon_n^{\text{CAN}}$ -reduced canonical domains $D_{\varepsilon,r}^n$, $r = 1, \dots, p$ and the $\varepsilon_n^{\text{CAN}}$ -reduced Stokes graph S_ε^n . In particular, the statement in Section A1.4 about the successful applications of the JWKB approximation modifies, in the presence of derivatives in the quantity (2.1) of Section 2, as follows:

A successful application of the JWKB approximation to solve any (global) one-dimensional quantum-mechanical problem requires the canonical properties 1.-4. of the fundamental solutions (stated in the Section A2.3) to remain valid also when the following substitutions is performed: $S \rightarrow S_\varepsilon^n$, $D_r \rightarrow D_{\varepsilon,r}^n$, $\psi_{D_r}^{(k)} \rightarrow C_k\psi_{D_r}^{\text{JWKB}}$, $K_{\varepsilon,D_r}^{\text{CAN}} \rightarrow K_{\varepsilon,D_r}^{\text{CAN}(n)}$, $k = 0, 1, \dots, n$, $r = 1, \dots, p$, with $\varepsilon_n^{\text{CAN}} \ll 1$.

The Stokes graph allowing such a JWKB approximation will be called as previously a JWKB approximation allowing graph.

For the sake of completeness let us write down also the following recurrent definitions of the coefficients α_k , a_k , b_k and d_k in (A1.18) and (A1.30):

$$\begin{cases} \alpha_k = \alpha'_{k-1} + \alpha \cdot \alpha_{k-1}, & k = 2, \dots \\ \text{with} \\ \alpha_0(x) \equiv 1, & \text{and} \quad \alpha(x) = -\frac{1}{4} \frac{Q'}{Q} + \sigma Q^{1/2}, \end{cases} \quad (\text{A1.37})$$

and

$$\begin{cases} a_k = a'_{k-1} + 2\sigma Q^{1/2} b_{k-1}, \\ b_k = b'_{k-1} - 2\sigma Q^{1/2} b_{k-1} + \sigma Q^{1/2} \omega d_{k-1}, \\ d_k = d_{k-1} - \sigma Q^{1/2} b_{k-1}, & k = 1, 2, \dots, \\ \text{with} \\ a_0 = d_0 = 0 \text{ and } b_0 = 1. \end{cases} \quad (\text{A1.38})$$

The function ω in (A1.38) is given by (A1.6).

As it follows from (A1.32), (A1.37) and (A1.38) a general structure of C_k in (A1.33) is the following:

$$C_k(x) = C_{k,1}(x) + \sigma Q^{1/2} C_{k,2}(x) \quad k = 0, 1, \dots \quad (\text{A1.39})$$

where $C_{k,i}$, $i = 1, 2$, are σ -independent rational functions of Q and q and their derivatives.

APPENDIX 2

We estimate here the accuracy of the approximate formula (3.10). For simplicity we shall do it for the case when $V_1 = V_2$, $E_1 = E_2$ and $M(x, d/dx) \equiv M(x)$.

It can be easily shown that the quantization condition for the energy E_1 in Fig. 1 takes the form:

$$iC_{1,L}\chi_{1,L \rightarrow U} = \exp[+iw_1^+(b_1)]C_{1,R}\chi_{1,R \rightarrow U}, \quad (\text{A2.1})$$

with $\chi_{1,X \rightarrow U} = \chi_{1,X}(\infty_U)$, $X = L, R$, and with the coefficient $\alpha_{1,L}$ in (3.8) given by:

$$\alpha_{1,L} = \chi_{1,L \rightarrow D} / \chi_{1,U \rightarrow D}. \quad (\text{A2.2})$$

Substituting the corresponding fundamental solutions into (3.8) and integrating the resulting series term by term we get:

$$\begin{aligned} \int_K \psi_1 M(x) \psi_1 dx &= C \left\{ \int_{\Gamma} + (\chi_{1,R \rightarrow D}^{(1)} + \chi_{1,L \rightarrow D}^{(1)} + \chi_{1,R \rightarrow U}^{(1)}) \int_{K_1} \right. \\ &\quad \left. + (\chi_{1,R \rightarrow D}^{(1)} + \chi_{1,L \rightarrow D}^{(1)} + \chi_{1,L \rightarrow D}^{(1)}) \int_{K_2} \right. \\ &\quad \left. + \int_{K_1} (\chi_{1,U}^{(1)} + \chi_{1,L}^{(1)}) + \int_{K_2} (\chi_{1,U}^{(1)} + \chi_{1,R}^{(1)}) \right\} \end{aligned}$$

$$\begin{aligned}
& -(\chi_{1,R \rightarrow U}^{(1)} + \chi_{1,L \rightarrow U}^{(1)} + \chi_{1,R \rightarrow D}^{(1)}) \int_{\bar{K}_1} \\
& -(\chi_{1,R \rightarrow U}^{(1)} + \chi_{1,L \rightarrow U}^{(1)} + \chi_{1,L \rightarrow D}^{(1)}) \int_{\bar{K}_2} \\
& - \int_{\bar{K}_1} (\chi_{1,D}^{(1)} + \chi_{1,L}^{(1)}) - \int_{\bar{K}_2} (\chi_{1,D}^{(1)} + \chi_{1,R}^{(1)}) \} Q_1^{-1/2} M(x) dx + \text{higher order terms}, \quad (A2.3)
\end{aligned}$$

where $\chi_{1,X}^{(1)}(x)$, $X = L, R, U, D$, $k = 1, 2$, are the first terms in the series (A1.8) and $C = i(C_{1,L})^2(\chi_{1,U \rightarrow D}\chi_{1,R \rightarrow U}\chi_{1,R \rightarrow D})^{-1}$ and the contour Γ is shown in Fig. 2.

Noticing now that $\chi_{1,U}^{(1)}(x) + \chi_{1,L}^{(1)}(x) \equiv \chi_{1,U \rightarrow L}^{(1)}$, $\chi_{1,U}^{(1)}(x) + \chi_{1,R}^{(1)}(x) \equiv \chi_{1,U \rightarrow R}^{(1)}$, ... etc. and putting $(\chi_{1,L \rightarrow D})^{-1} = 1 - \chi_{1,L \rightarrow D}^{(1)} + \dots$, etc. we get from (A2.3):

$$\begin{aligned}
& \int_K (\psi_1)^2 M(x) dx = i(C_{1,L})^2 (1 + \chi_{1,L \rightarrow D}^{(1)}) \\
& - \chi_{1,U \rightarrow D}^{(1)} + \chi_{1,L \rightarrow U}^{(1)} \int_{\Gamma} Q_1^{-1/2} M(x) dx + \text{higher order terms}. \quad (A2.4)
\end{aligned}$$

Noticing further that

$$|\chi_{1,L \rightarrow D}^{(1)} - \chi_{1,U \rightarrow D}^{(1)} + \chi_{1,L \rightarrow U}^{(1)}| = |\frac{1}{2} \int_{\Gamma_1} \omega_1(x) Q_1^{1/2} dx| \leq \frac{3}{2} \epsilon^{\text{CAN}}, \quad (A2.5)$$

where the contour Γ_1 is shown in Fig. 2, we see that ϵ^{CAN} provides the proper measure of the accuracy of the approximation (3.10).

APPENDIX 3

We estimate here the left-hand side of (A1.19) for $\chi_{E_0, L \rightarrow U'}$ and show that it cannot be fulfilled by any $\epsilon < 1$. To do this let us consider the integral (see Fig. 12):

$$I_\delta = \int_{x_+ - \delta}^{x_+ + \delta} \omega(x) Q^{1/2} dx, \quad (A3.1)$$

where $\omega(x)$ is defined by the superpotential $U(x) = x(x^2 - \alpha^2)$ with the help of (A1.6) (where $Q(x) \equiv q(x) = [(U')^2 - \hbar U'' - 2E_0]/\hbar^2$). Noticing that in the vicinity of the point $x_+ = -\alpha/\sqrt{3}$ we can write $q = 9(x-c)(x-\bar{c})(x-a)(x-b)/\hbar^2 \approx 9(x_+ - x_-)^2[(x - x_+)^2 + \delta^2]/\hbar^2$ we get for I_δ :

$$\begin{aligned}
I_\delta & \cong (\hbar/4) [2 \int_{-1}^1 (1+x^2)^{-1/2} dx - 5 \int_{-1}^1 x^2 (1+x^2)^{-1/2} dx] / [(x_+ - x_-)\delta^2] \\
& = -[7\sqrt{2} - 3 \ln(1 + \sqrt{2})]/4 = -1.8. \quad (A3.2)
\end{aligned}$$

It follows from (A3.2) that the condition (A1.19) cannot be fulfilled for $x \rightarrow \infty_{U'}$, i.e. that we cannot put $\chi_{E_0, L \rightarrow U'}^{\text{JWKB}} = 1$.

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