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Generalised WKBJ formulae

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Abstract. An infinite sequence of new representations having Fröman and Fröman's form has been found for the solutions to the one-dimensional Schrödinger equation (SE). This enables us to construct, in compact WKBJ-like form, approximate solutions to SE. The new approximate solutions have the property that their asymptotic expansions in $\hbar$ coincide with the corresponding asymptotic expansions of the exact solutions to any, *a priori* given, order in $\hbar$. They generalise the well known WKBJ formula, being in this scheme the zeroth-order approximation. The generalised WKBJ formulae are then tested by the quantisation of the simplest quantum mechanical systems of the harmonic and anharmonic (quartic) oscillators as well as a more complicated one of a double-well potential. The approximate quantisation rules (a generalisation of the well known Bohr-Sommerfeld quantisation conditions) for the general polynomial potential is finally obtained and the formulae for calculating the necessary corrections are derived. The limiting formal solutions to SE having the WKBJ form are also presented. Their asymptotic expansions in $\hbar$ reproduce those found by Fröman.

1. Introduction

The WKBJ formula (Wentzel 1926, Kramers 1926, Brillouin 1926, Jeffreys 1923, Dunham 1932) provides us with rather simple and surprisingly good approximate solution to the SE. For this reason it is widely used in many approximate calculations of quantum mechanical quantities (see, for example, Berry and Mount 1972, Hioe *et al* 1978), especially if the problem under consideration cannot be handled by more common perturbative calculations. Different tunnelling effects, as well as other effects caused by potential barriers (e.g. the tiny effect of the ground-state energy in the case of a quantum mechanical potential with broken supersymmetry (Giler *et al* 1986)), are examples in which the use of the WKBJ formula gives correct results.

However, there are always theoretical efforts to improve the accuracy of the WKBJ approximation. On one side, these include the direct modification of the WKBJ formula (Fröman 1966, Fröman and Fröman 1974a, b) and on the other side new methods are being developed to investigate the asymptotic behaviour of the solutions to the SE (Balian *et al* 1979, Voros 1983).

From the mathematical point of view the WKBJ formula has two distinct features.

(i) It is a well defined dominant term of the exact solution to the SE, whose accuracy can be determined precisely (Fröman and Fröman 1965).

(ii) It generates the zeroth-order term of the asymptotic series in $\hbar$, which corresponds to the exact solution to the SE.

An important generalisation of the WKBJ formula has been found by Fröman (1966) (see also Fröman and Fröman (1974a, b) for later modifications). It preserves the

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compact form of the WKBJ formula and has the same asymptotic expansion in $\hbar$ as the exact solution to the SE. However, Fröman's formula, which was argued to be very useful in applications (see Dammert and Fröman (1980) for relevant discussion and references), has, from our point of view, at least two main disadvantages. Firstly, the formula is constructed with the help of an asymptotic series, which, in most cases, is divergent. Therefore to give finite quantities the series has to be truncated. Secondly, it is usually very difficult to estimate the level of the accuracy for quantities obtained in such a way, since the truncated formula constitutes an unknown part of the exact solution to the SE. It seems therefore to be useful to find such approximate solutions to the SE, which

(i) would have as compact a form as the WKBJ one;

(ii) would be a well defined dominant term of the exact solution to the SE; and

(iii) would differ asymptotically from the exact solutions to an *a priori* given order in $\hbar$.

It is the aim of this paper to show that such generalisations of the WKBJ formula do exist and to give an algorithm for their construction.

To achieve the purposes stated above we use extensively a method which consists in changing the variable in the SE repeatedly and in using the Fröman and Fröman (FF) form of the solutions to the new equations (Fröman and Fröman 1965). In fact, the variables which we use consecutively in the SE are the action variables. They transform the equation preserving its form. This enables us to construct each time the corresponding solutions to the new equations in the form of the FF series, the first term of which represents the approximate solutions with the desired properties.

The paper is organised as follows. In the next section the solutions to the SE in the FF form are given and their main properties are summarised. In § 3 we construct approximate solutions to the SE with desired properties. In § 4 the approximate solutions obtained in § 3 are applied to a 'school' example of the harmonic oscillator as well as to an anharmonic (quartic) one. We show that the energy spectra in the case of the harmonic oscillator are the same, independent of the approximation we use and coincide with the energy spectrum given by the commonly used WKBJ formula, i.e. they are exact. In the same section we consider also the case of a double-well potential given by a polynomial of the sixth degree. Having considered these particular examples we investigate finally the general case. In § 5 we present explicitly the exact solutions to the SE having the WKBJ form but being rather formal ones and we explain their asymptotic meanings. However, we find that the asymptotic form in $\hbar$ for these solutions reproduces those found by Fröman (1966). We also discuss in this section the problem of the resummation arising due to the FF forms of the solutions. We conclude with § 6.

2. Fröman and Fröman's form of the solution to the SE

To simplify our further considerations and to make them more definite, we shall assume that the potential $U(x)$ in the SE is just a polynomial of the degree $2n$, $n = 1, 2, \ldots$, with real coefficients. This restriction is, however, not very serious and can be relaxed in many physically interesting cases (such as the case of the Coulomb potential, for example). Let us now write the (one-dimensional) Schrödinger equation in the form

$$\phi''(x) - Q(x)\phi(x) = 0 \tag{1}$$

where

$$Q(x) = 2m[U(x) - E]/\hbar^2$$
$$U(x) = a_{2n}x^{2n} + a_{2n-1}x^{2n-1} + \ldots + a_1 x + a_0$$

with $a_{2n} > 0$.

It is convenient in (1) to make a replacement $x \to x(E/a_{2n})^{1/2n}$. Putting also $\alpha^2 = 2mE^{(n+1)/n}/(\hbar^2 a_{2n}^{1/n})$, $V(x, E) \equiv U(x(E/a_{2n})^{1/2n})/E$, $q(x) \equiv V(x) - 1$ and $\psi(x) \equiv \phi(x(E/a_{2n})^{1/2n})$ we get

$$\psi''(x) - \alpha^2 q(x)\psi(x) = 0. \tag{2}$$

Note that the variables x and α are dimensionless. By making the ansatz

$$\psi_\sigma(x) = q^{-1/4}(x) \exp[\sigma S(\xi^0, x)]\tilde{\psi}_\sigma(x) \qquad \sigma = \pm 1 \tag{3}$$

where

$$S(x^0, x) \equiv x_1(x^0, x) = \alpha \int_{x^0}^{x} q^{1/2}(\xi)\, \mathrm{d}\xi$$
$$q(x^0) = 0 \tag{4}$$

we obtain the appropriate equation determining $\tilde{\psi}_\sigma(x)$. Solving by iteration we get

$$\tilde{\psi}_\sigma(x) = 1 + \sum_{n \geq 1} (\tfrac{1}{2}\sigma)^n \int_{\gamma^\sigma(x_1)} \mathrm{d}\xi_1 \int_{\gamma^\sigma(\xi_1)} \mathrm{d}\xi_2 \ldots \int_{\gamma^\sigma(\xi_{n+1})} \mathrm{d}\xi_n [q_1(\xi_1) - 1] \ldots [q_1(\xi_n) - 1]$$
$$\times \{1 - \exp[2\sigma(\xi_2 - \xi_1)]\} \ldots \{1 - \exp[2\sigma(\xi_n - \xi_{n-1})]\} \tag{5}$$

where

$$q_1(x_1) = 1 + \frac{1}{4\alpha^2}\left(\frac{q''(x)}{q^2(x)} - \frac{5}{4}\frac{q'^2(x)}{q^3(x)}\right). \tag{6}$$

In equation (5) the path $\gamma^\sigma(\xi_i)$ of the integrations starts from the infinity of the x plane and goes to ξ_i in such a way so as to ensure that Re ξ_{i+1} changes monotonically everywhere along the path, as well as to have Re $\sigma(\xi_{i+1} - \xi_i) \leq 0$ along the path. The series in (5) is uniformly convergent under the condition that

$$\inf \int_{\gamma^\sigma(x_1)} |q_1(\xi) - 1||\mathrm{d}\xi| < \infty \tag{7}$$

for the paths $\gamma^\sigma(x_1)$ chosen as above. It is easy to check that (7) is satisfied by our choice of $U(x)$.

Let us discuss briefly the dependence of the series (5) on $\hbar$. If $U(x)$ is independent of $\hbar$ then the nth term ($n \geq 0$) of the series (5) being proportional to α^{-n} simultaneously has the factor $\hbar^n$. Of course, it does not mean that the term has no additional dependence on $\hbar$, but when $\hbar \to 0$ this term vanishes at least as $\hbar^n$. It therefore contributes to the nth term of the corresponding asymptotic series for the solution (3).

A convenient way to describe the validity domains of the representations (3) and (5) is to draw the so-called Stokes' graph (SG). Such a graph consists of Stokes' lines (SL) given by the equation Re $S(x^0, x) = 0$ for all roots x^0 of $q(x)$. Every system of SL divides the whole complex x plane into the set of disjoint sectors. Solutions of the form given by (3) and (5) can be constructed in each sector which contain $+\infty$ or $-\infty$ of Re $S(x^0, x)$ and in each such sector it is uniquely (up to a constant) determined by

the condition of vanishing as $x \to \infty$ in this sector. It can be analytically continued (with the help of the representation (3)-(5)) to those other sectors to which the integration path can be continued. In all such sectors it grows exponentially. Moreover, any two solutions of the form (3)-(5) corresponding to different sectors are linearly independent. This fact is the obvious consequence of their asymptotic behaviour described above.

3. Approximate solutions to SE to a given order of accuracy

The usual WKBJ formula follows directly from the solution (3) if instead of (7) we have

$$\inf \int_{\gamma^{\sigma}(x_1)} |q_1(\xi) - 1||\mathrm{d}\xi| \ll 1. \tag{8}$$

The condition (8) can be satisfied if α is sufficiently large, at fixed x, and if by increasing α we do not change the picture of the corresponding Stokes' graph. It means that

(i) the WKBJ formula works well for rather high energy levels; and

(ii) it constitutes the zeroth-order term of the asymptotic series for the solution (3).

Let us notice that if $\alpha \to \infty$ (at fixed x) the variable $S(x^0, x)$ as defined by (4) also grows to infinity. So the action S seems to be a very convenient variable when the WKBJ formula is investigated.

The choice of the action as the new variable in the SE also has another useful property: it does not change the form (2) of the SE. To see this, let us define the following new quantities:

$$\begin{aligned}
&\tilde{q}(x_1) \equiv \alpha^2 q(x) \\
&\phi_0(x_1) \equiv \psi(x) \\
&\psi_1(x_1) = \tilde{q}^{1/4}(x_1)\phi_0(x_1) \\
&q_1(x_1) = 1 + \frac{1}{4}\left(\frac{\tilde{q}''(x_1)}{\tilde{q}(x_1)} - \frac{3}{4}\frac{\tilde{q}'^2(x_1)}{\tilde{q}^2(x_1)}\right) \\
&\qquad = 1 + \frac{1}{4\alpha^2}\left(\frac{q''(x)}{q^2(x)} - \frac{5}{4}\frac{q'^2(x)}{q^3(x)}\right)
\end{aligned} \tag{9}$$

where x_1 is defined by (4). It is straightforward to check that $\psi_1(x_1)$ now satisfies the equation

$$\psi_1''(x_1) - q_1(x_1)\psi_1(x_1) = 0 \tag{10}$$

which, of course, is formally the same as (2). Obviously, the main difference between them is now in the domains, where the functions $q(x)$ and $q_1(x_1)$ are defined. For the first one it is simply, by assumption, the x plane. For the second, however, it can be a complicated Riemann surface, which arises as the result of the transformation (4). No matter how complicated the surface is, we can always write the solution $\psi_1(x_1)$ of (10) in the FF form (3) and (5) with appropriate definitions of the quantities (4) and (6). This is possible since, by our assumptions about $U(x)$, an analogue of the condition (7) is also fulfilled in the case of equation (10) (see appendix 1). Similarly, drawing the corresponding SL on the Riemann surface of the x_1 variable, we get the domains where the solutions $\psi_1(x_1)$ are defined.

It is now clear that the above procedure can be continued inductively with the kth step being

$$\begin{aligned}
&q_{k-1}(x_{k-1}^0) = 0 \\
&x_k(x_{k-1}^0, x_{k-1}) = \int_{x_{k-1}^0}^{x_{k-1}} q_{k-1}^{1/2}(\xi)\,\mathrm{d}\xi \\
&\phi_{k-1}(x_k) \equiv \psi_{k-1}(x_{k-1}) \\
&\tilde{q}_{k-1}(x_k) = q_{k-1}(x_{k-1}) \\
&\psi_k(x_k) = \tilde{q}_{k-1}^{1/4}(x_k)\phi_{k-1}(x_k) \\
&q_k(x_k) = 1 + \frac{1}{4}\left(\frac{\tilde{q}_{k-1}''(x_k)}{\tilde{q}_{k-1}(x_k)} - \frac{3}{4}\frac{\tilde{q}_{k-1}'^2(x_k)}{\tilde{q}_{k-1}^2(x_k)}\right) \\
&\qquad = 1 + \frac{1}{4}\left(\frac{q_{k-1}''(x_{k-1})}{q_{k-1}^2(x_{k-1})} - \frac{5}{4}\frac{q_{k-1}'^2(x_{k-1})}{q_{k-1}^3(x_{k-1})}\right)
\end{aligned} \tag{11}$$

and

$$\psi_k''(x_k) - q_k(x_k)\psi_k(x_k) = 0. \tag{12}$$

We have made the following identification with the quantities introduced earlier (see (2) and (9)):

$$\begin{aligned}
&x_0 \equiv x \qquad\qquad \psi_0(x_0) \equiv \psi(x) \\
&\tilde{q}_0(x_1) \equiv \tilde{q}(x_1) \qquad\qquad q_0(x_0) \equiv \alpha^2 q(x).
\end{aligned} \tag{13}$$

The solution of (12) can be written in the FF form as follows:

$$\psi_k^\sigma(x_k) = q_k^{-1/4}(x_k)\exp[\sigma x_{k+1}(x_k^0, x_k)]\tilde{\psi}_k^\sigma(x_k) \qquad \sigma = \pm 1 \tag{14}$$

with $\tilde{\psi}_k^\sigma(x_k)$ defined by (5) and (6) where obvious changes of variables ($x_1 \to x_{k+1}$, $q_1 \to q_{k+1}$) and integrations (over the x_{k+1} Riemann surface) should be done. The existence of the solutions ψ_k^σ in the form (14) is guaranteed at each step by our assumption about $U(x)$, since the condition (7) is satisfied for any $k \geqslant 0$ (see appendix 1). The validity domain of every particular solution (14) is controlled by appropriate SG drawn on the x_k surface.

Now let us come back to the main object of our interest, namely to the wavefunction $\psi(x)$—the solution of the SE (2). Using the definitions (9), (10) and (13) we get

$$\begin{aligned}
\psi_\sigma(x) = &[q(x)q_1(x_1(x)) \ldots q_k(x_k(x))]^{-1/4} \\
&\times \exp\left(\sigma\alpha \int_{\xi_k^0}^{x} [q(\xi)q_1(x_1(\xi)) \ldots q_k(x_k(\xi))]^{1/2}\,\mathrm{d}\xi\right)\tilde{\psi}_k^\sigma(x_k(x))
\end{aligned} \tag{15}$$

where $x_i(x)$ is the composition $x_i = x_{i-1} \circ x_{i-2} \circ \ldots \circ x_1$, $i = 1, \ldots, k$, of the appropriate transformations defined by (11), and ξ_k^0 is the projection of x_k^0 onto the x plane, i.e. $x_k(\xi_k^0) = x_k^0$.

Of course all other properties of the solutions $\psi_k^\sigma(x_k)$ are also projected onto the x plane. In particular, the validity domain of the representation (15) is given by SG in the x plane, defined as a set of lines along which $\mathrm{Re}\, S_k(\xi_k^0, x) = 0$, with S_k given by

$$S_k(\xi_k^0, x) = \alpha \int_{\xi_k^0}^{x} [q(\xi)q_1(x_1(\xi)) \ldots q_k(x_k(\xi))]^{1/2}\,\mathrm{d}\xi \tag{16}$$

for all choices of the roots ξ_k^0 of the equation $q_k(x_k(\xi_k^0)) = 0$.

We shall call the forms (15) of the solutions to the SE, with k fixed, their kth FF forms. The Stokes' graph corresponding to the kth FF forms we shall call the kth Stokes' graph.

The most striking feature of the representation (15) (when $U(x)$ is independent of $\hbar$) is that the nth term ($n \geqslant 1$) of the series (5), corresponding to $\tilde{\psi}_k^{\sigma}(x_k)$, is proportional to α^{-2k-n} and therefore to $\hbar^{2k+n}$ (see appendix 2). It follows then immediately that the expression

$$\chi_k^{\sigma}(x) = [q(x)q_1(x_1(x)) \ldots q_k(x_k(x))]^{-1/4} \exp[\sigma S_k(\xi_k^0, x)] \tag{17}$$

satisfies equation (2) approximately under the assumption (see appendix 4)

$$\inf \int_{\gamma_k(x_k(x))} |q_{k+1}(x_{k+1}(\xi)) - 1||qq_1 \ldots q_k|^{1/2} |\mathrm{d}\xi| \ll 1. \tag{18}$$

Since the LHS of (18) contains the factor α^{-2k-1}, the above inequality seems to be satisfied much better than (8) for the same energy. In other words, the approximation (17) can be good even for those lower lying energy states for which the usual WKBJ formula fails.

Another good property of (17) is that its asymptotic series in $\hbar$ is identical, up to order $\hbar^{2k}$, with that of the exact solution (15).

Equation (17) therefore has the main properties we are looking for. It can be constructed for any integral $k \geqslant 0$ starting with the conventional WKBJ approximation. So, it represents the natural generalisation of the latter. Therefore we shall call the approximations (17) for fixed k the kth WKBJ formulae (or the kth WKBJ approximations).

At each step of constructing the solutions (15) and their approximations (17) we have chosen a particular root of the current potential to define a new subsequent variable for the transformed equation (see (11) and (12)). Therefore the question might arise whether different choice of the roots could affect the final results of the procedure (see equations (15)–(17)), i.e. whether we could get other solutions of the form (15) with, correspondingly, other SG by choosing another set of roots in the intermediate steps.

The negative answer to this question is contained in the final form of the solutions (15). Each quantity from the solution (15) is constructed only from the function $(qq_1 \ldots q_k)(x)$ and its integrals. The function $(qq_1 \ldots q_k)(x)$ alone is independent of the choice of the roots in any step of the construction procedure since it is obtained locally from the function q and its derivatives by algebraic operations (see (11)).

The action S_k depends only on the roots of $(qq_1 \ldots q_k)(x)$, i.e. on the final choice of one of them. However, as follows from (16), any two different choices of the root can change S_k only by a constant. Of course this cannot influence the SG since it is drawn by making use of all the roots of $(qq_1 \ldots q_k)(x)$.

Finally, the functions $\tilde{\psi}_k(x_k(x))$ do not depend at all on the choice of the roots in the intermediate steps, by their definition (5) for the following reasons: firstly, because any such choice does not affect SG and this is crucial for the definition of $\tilde{\psi}_k(x_k(x))$; and secondly, because the integrands in (5) depend on $(qq_1 \ldots q_k)(x)$ and its derivatives algebraically and the action S occurs there only in the form of differences.

Therefore the conclusion is that any other choice of a set of roots always leads to the same set of the solutions (15) (if one neglects possible multiplicative constants arising from different definitions of S_k).

Another question that can arise is connected with possible relations between the solutions having different FF forms. However, the discussion of this topic is left to § 5, after presenting the results of particular applications of the formulae (15) and (17).

4. The harmonic and anharmonic (quartic) oscillators and the double-well potential quantised by generalised WKBJ formulae

To see the main difference (but also similarities) between the applications of the usual WKBJ formula and its generalisations we shall first sketch the way of using the former for the harmonic and quartic oscillators, as well as for the double-well potential and next describe the use of the generalised formulae.

The general prescription for using both the usual and generalised WKBJ formulae is to remember that:

(i) they are approximate solutions to the SE given in FF forms, so they can be used only in the appropriate domains of their validity given by the corresponding Stokes' graph; and

(ii) any two of them defined in their appropriate regions should be regarded formally as linearly independent (although in fact they are not); on the other hand, any of them can be (formally) expressed as a linear combination of any two others.

4.1. The harmonic oscillator case

The Stokes's graph for the usual WKBJ formula is shown for this case in figure 1 ($q(x) = x^2 - 1$). Let χ_k, $k = 1, 2, \bar{2}, 3$, denote the WKBJ formulae for the appropriate regions of the graph. The quantisation condition then becomes

$$\chi_1(x) = C\chi_3(x) \tag{19}$$

where C is a (real) constant. Both χ_1 and χ_3 can be continued to the regions 2 and $\bar{2}$ and therefore the constant C can be calculated as follows:

$$C = \lim_{x \to \infty_2} \frac{\chi_1(x)}{\chi_3(x)} = \lim_{x \to \infty_{\bar{2}}} \frac{\chi_1(x)}{\chi_3(x)}. \tag{20}$$

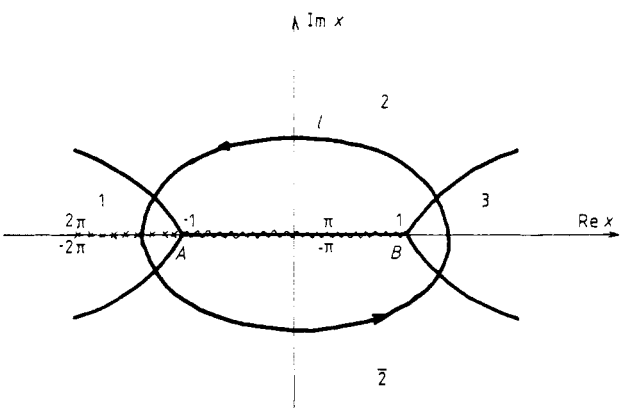

Figure 1. The zeroth SG for the harmonic oscillator.

Taking into account that

$$\chi_1 = \mathrm{i} q^{-1/4} \exp[-S(-1, x)]$$

$$\chi_3 = q^{-1/4} \exp[-S(1, x)]$$

we get

$$C = \mathrm{i} \exp[-S_+(-1, 1)] = -\mathrm{i} \exp[\ -S_-(-1, 1)] \tag{21}$$

where '±' at $S_\pm(-1, 1)$ denote the integrations above or below the cut $(-1, 1)$, respectively. Equations (21) can be satisfied and the constant C can be real, if

$$\exp\left(-\alpha \oint_I q^{1/2}\, \mathrm{d}\xi\right) = -1 \tag{22a}$$

or

$$-\frac{\alpha}{\mathrm{i}} \oint_I q^{1/2}\, \mathrm{d}\xi = (2n+1)\pi. \tag{22b}$$

Equation (22*b*) is the usual Bohr–Sommerfeld quantisation condition giving the well known exact energy spectrum in the case considered.

What happens if we use the next approximate solution (17) (in the sequence)? Firstly, it changes the Stokes' diagram (figure 2), since a new $(\alpha^2 q q_1)(x)$ is now

$$(\alpha^2 q q_1)(x) = \alpha^2 \left[x^2 - 1 + \frac{1}{4\alpha^2} \left(\frac{2}{x^2-1} - \frac{5x^2}{(x^2-1)^2} \right) \right]. \tag{23}$$

The function $(\alpha^2 q q_1)(x)$ now has zeros at the points A_1, C_1, $\bar{C}_1$, and B_1, D_1, $\bar{D}_1$ (at a distance proportional to $\hbar^{2/3}$ from the points $(-1, 0)$, $(1, 0)$ respectively) and poles at the points $(-1, 0)$, $(1, 0)$. The number of independent solutions remains the same as well as does the quantisation procedure (19)–(22), where one needs to only change q into qq_1. So the quantisation condition now becomes

$$-\frac{\alpha}{\mathrm{i}} \oint_{I_1} (qq_1)^{1/2}(\xi)\, \mathrm{d}\xi = (2n+1)\pi \tag{24}$$

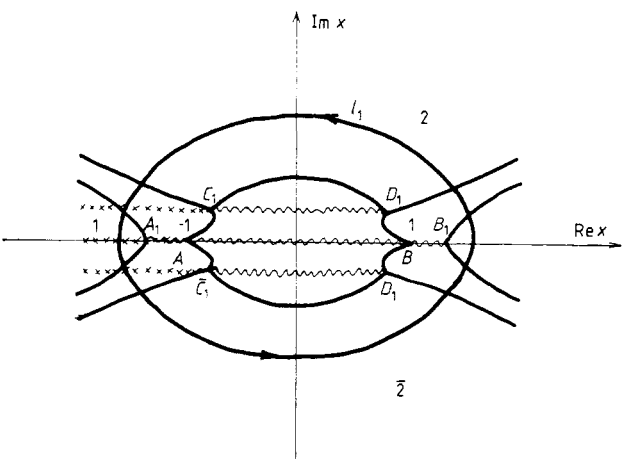

Figure 2. The first SG for the harmonic oscillator.

where l_1 is shown in figure 2. Does this new formula give a result different from (22)? To evaluate the integral in (24), we use the residue theorem to get

$$-\frac{\alpha}{i}\oint_{l_1}(qq_1)^{1/2}(\xi)\,d\xi=\pi\alpha=2\pi E/\hbar \tag{25}$$

since outside the contour l_1, $(qq_1)^{1/2}$ is meromorphic with a simple pole at the infinity. So the result for the energy spectrum is the same as before.

It is now also clear what result will be obtained with the help of the kth approximation (17). The kth SG should look as in figure 3. The additional SL appearing in the figure and running to infinity cannot produce new domains with new solutions since the graph in figure 3 must collapse into the graph in figure 1 if $\hbar\to 0$. For the same reason, the blob in the centre of figure 3 contains all singularities of the function $(qq_1\ldots q_k)(x)$ and all the cuts of $(qq_1\ldots q_k)^{1/2}(x)$ (except those shown explicitly in figure 3). Therefore the quantisation condition still remains the same:

$$-\frac{\alpha}{i}\oint_{l_k}(qq_1\ldots q_k)^{1/2}(\xi)\,d\xi=(2n+1)\pi \tag{26}$$

and the evaluation of its LHS (easily done as before) gives the same result (25).

Thus the conditions (22), (25) and (26), although obtained as approximate, give the same result for the energy spectrum. Moreover, this result is exact. It should not, however, be unexpected since, in fact, all these conditions are exact, i.e. they would remain unchanged if we used the exact solutions (15) (instead of their approximations (17)) in the quantisation procedure to get them. Of course, it is not true in general.

The striking common feature of the conditions (22), (24) and (26) is their identical Bohr-Sommerfeld form. It is therefore natural to call (26) the kth generalised Bohr-Sommerfeld condition (kth GBS condition).

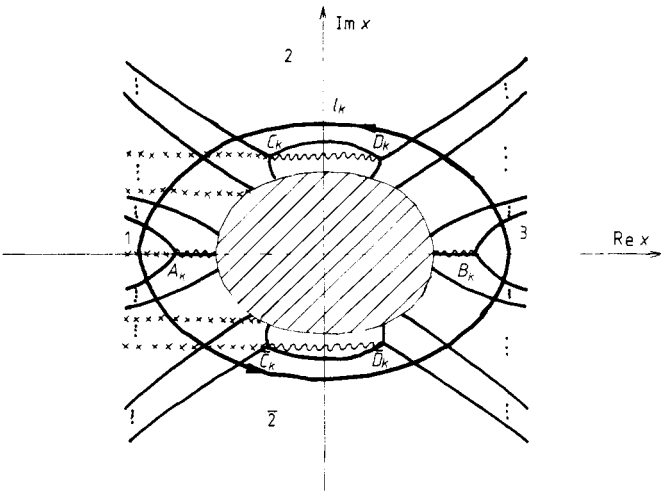

Figure 3. The kth SG for the harmonic oscillator.

4.2. The anharmonic (quartic) oscillator case

As a second example let us consider the potential $U(x)=x^4$. For the zeroth approximation (17) ($k=0$) the SG looks as in figure 4. Following the previous procedure we get

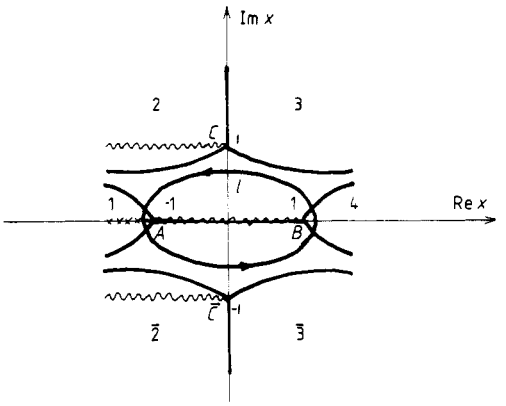

Figure 4. The zeroth SG for the quartic oscillator.

the quantisation condition as in (22) where now $q(x)=x^4-1$, $\alpha^2=2E^{3/2}/\hbar^2$ and the contour l is shown in figure 4. The (trivial) solution to this condition is

$$E_n=\frac{1}{4}\left[\pi(n+\tfrac{1}{2})\hbar\left(\int_0^1(1-\xi^4)^{1/2}\,\mathrm{d}\xi\right)^{1/2}\right]^{4/3}=0.94[(n+\tfrac{1}{2})\hbar]^{4/3}. \tag{27}$$

The above formula is valid for those E_n which satisfy additionally the following inequality (see (19) and appendix 4):

$$\frac{1}{(2n+1)\pi}\left|\oint_l(1-x^4)^{1/2}\,\mathrm{d}x\oint_l\left(\frac{3x^2}{(x^4-1)^{3/2}}-\frac{5x^6}{(x^4-1)^{5/2}}\right)\mathrm{d}x\right|\ll 1. \tag{28}$$

Performing integrations in (28) we get the following estimation for n, for which (27) is valid: $n\gg -0.17$.

Let us now take into account the next ($k=1$) approximation (17). The function $(qq_1)(x)$ for that case is

$$(qq_1)(x_1)=x^4-1+\frac{1}{\alpha^2}\left(\frac{3x^2}{x^4-1}-\frac{5x^6}{(x^4-1)^2}\right) \tag{29}$$

and the corresponding SG are presented in figure 5. The quantisation rule has the form

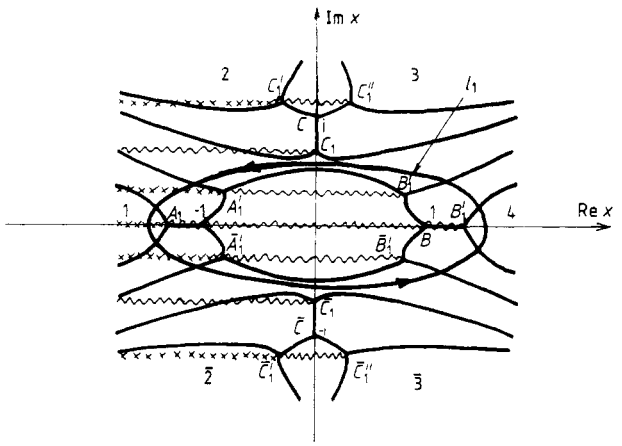

Figure 5. The first SG for the quartic oscillator.

(24) under the condition:

$$\left|\oint_{l_1} \alpha(q_2-1)(qq_1)^{1/2}\,\mathrm{d}\xi\right| \ll 1 \tag{30}$$

where now $\alpha|q_2-1|$ is proportional to α^{-3} (note however that the whole integrand in (30) has additional dependence on α^{-1}, analytic when $\alpha\to\infty$).

To get the improved energy spectrum we should, of course, perform the integration in the quantisation formula (24). Perhaps the simplest way to do this is the numerical one. However, to get the asymptotic expression for the energy levels (when $\alpha\to\infty$) to the order α^{-2} (because of (30)) we should simply expand the integrand in (24) into the power series in α^{-1} and terminate it at α^{-2} term. In this way we obtain

$$\alpha\left(-\frac{1}{\mathrm{i}}\oint_l q^{1/2}\,\mathrm{d}\xi\right)+\frac{1}{\alpha}\left[-\frac{1}{\mathrm{i}}\oint_l \frac{1}{2}\left(\frac{3\xi^2}{(\xi^4-1)^{3/2}}-\frac{5\xi^6}{(\xi^4-1)^{5/2}}\right)\mathrm{d}\xi\right]=(2n+1)\pi \tag{31}$$

where we have changed the contour l_1 from figure 5 into the one from figure 4, because, due to our expansion, all the singularities at the points A_1, A_1', $\overline{A_1'}$ and B_1, B_1', $\overline{B_1'}$ have disappeared. The solution to (31) is

$$\begin{aligned} E_n' &= [\pi(n+\tfrac{1}{2})\hbar/I_1 - I_2/(2n+1)\pi]^{4/3} \\ &\approx E_n\left(1-\frac{1.2\times 10^{-3}}{(n+\frac{1}{2})^3}\right) \end{aligned} \tag{32}$$

where E_n is given by (27) and I_1, I_2 are the first and the second integrals on the LHS of (31), respectively.

It is clear from the above how to proceed further in the case considered. The kth SG is shown in figure 6. The kth GBS quantisation rule associated with SG of figure 6 is

$$-\frac{\alpha}{\mathrm{i}}\oint_{l_k}(qq_1\ldots q_k)^{1/2}\,\mathrm{d}\xi=(2n+1)\pi \tag{33}$$

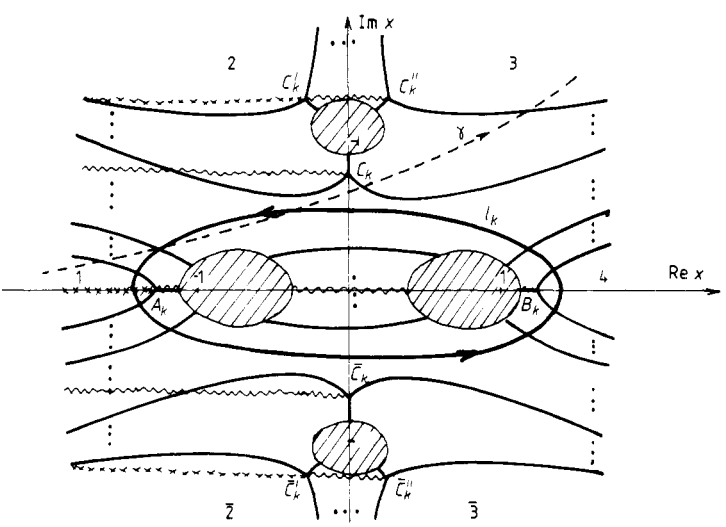

Figure 6. The kth SG for the quartic oscillator.

together with the condition (see appendix 4):

$$\left|\alpha \oint_{l_k} (q_{k+1}-1)(qq_1 \ldots q_k)^{1/2}\, d\xi\right| \ll 1. \tag{34}$$

As explained earlier the LHS of (34) is proportional to α^{-2k-1}, i.e. to $\hbar^{2k+1}/E^{(2k+1)(n+1)/n}$ ($2n$ is the degree of the polynomial $U(x)$), and therefore the greater k is in (33) the lower the energies needed to satisfy (34).

In order to get the asymptotic condition for the energy levels when $\alpha \to \infty$, valid to order α^{-2k}, we should expand the integrands in (33) into the power series in α^{-1} and truncate it on the power α^{-2k}. Then all the integrations at (33) reduce to the ones made around the cut AB of figure 4, since all the other singularities contained in the blobs of figure 6 disappear due to the expansion. The integrations depend on the energy E as the parameter and if they are performed one gets the equations for the energy levels in the involved form. Now to invert them remains a problem of the method.

4.3. A double-well potential

In order to see how to proceed in the case of many-well potentials we shall examine the potential of the form:

$$q(x) = V(x) - 1 = (x-a)(x-b)(x-c)(x-d)[(x-f)^2+g^2] \tag{35}$$

where $a < b < 0 < c < d$ and $f, g > 0$. The potential (35) has therefore two wells and two complex conjugate turning points. Of course, all its roots are functions of the energy E.

Performing the quantisation procedure in the case considered, we shall first derive exact quantisation rules for the energy using the exact solutions (15) and next we shall discuss their corresponding approximations obtained with the help of the formulae (17).

Let ψ_k, $k = 0, 1, \ldots$, be the solutions of the SE having the kth FF forms and corresponding to the potential of (35). We shall consider subsequently the cases $k = 0, 1$ and then an arbitrary k.

4.3.1. $k = 0$. The SG for this case is shown in figure 7. Let ψ_{0p}, $p = 1, 2, \bar{2}, 4, \bar{4}, 5$, be the corresponding solutions. The quantisation procedure consists as usual of matching

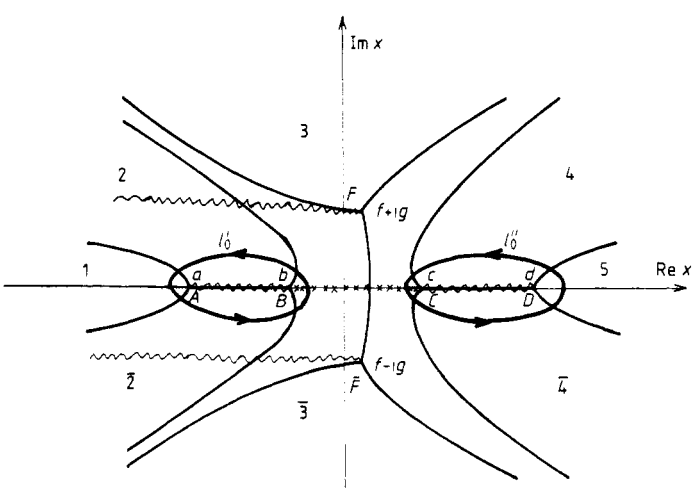

Figure 7. The zeroth SG for the double-well potential.

the wavefunction ψ_{01} defined in the sector 1 with ψ_{05} defined in 5. However, in the considered case, in contrast to the previous ones, there is no common domain to which both the solutions can be continued, preserving their FF forms. Therefore to match them it is necessary to use the solutions ψ_{0p} with $p = 2, \bar{2}, 4, \bar{4}$. The corresponding procedure has been performed in appendix 3. The exact quantisation formula can be written in the form

$$\left[1+\exp\left(\alpha \oint_{l_0'} q^{1/2}\,\mathrm{d}\xi + \mathrm{i}\delta^0_{2\to 4} + \mathrm{i}\delta^0_{2\to\bar{4}}\right)\right]\left[1+\exp\left(-\alpha \oint_{l_0''} q^{1/2}\,\mathrm{d}\xi - \mathrm{i}\delta^0_{2\to 4} + \mathrm{i}\delta^0_{2\to\bar{4}}\right)\right]$$
$$= \rho^0 \exp[2S_0(b, c)] \tag{36}$$

where ρ^0 is given by

$$\rho^0 = -2\frac{\tilde{\psi}^0_{2\to\bar{2}}\tilde{\psi}^0_{4\to\bar{4}}}{|\tilde{\psi}^0_{2\to 4}|^2}\left[1+\left(1+\frac{\tilde{\psi}^0_{2\to\bar{2}}\tilde{\psi}^0_{4\to\bar{4}}}{|\tilde{\psi}^0_{2\to 4}|^2}\exp[2S_0(b, c)]\right)^{-1/2}\right]^{-1}\cos\alpha_-$$
$$\times\exp\left(\tfrac{1}{2}\alpha\oint_{l_0'} q^{1/2}\,\mathrm{d}\xi - \tfrac{1}{2}\alpha\oint_{l_0''} q^{1/2}\,\mathrm{d}\xi + \delta^0_{2\to\bar{4}}\right) \tag{37}$$

and the meaning of each quantity in (36) and (37) is defined in appendix 3. Note that $S_0(b, c) < 0$.

How does the formula (36) change if we use the WKBJ approximations? We should put formally $\tilde{\psi}_{0p}(x) \equiv 1$ for any $p = 1, 2, \ldots, 5$. This means that we can obtain the corresponding approximate quantisation condition from (36) putting its RHS, and all the phases $\delta_{i\to j}$ appearing there, equal to zero. Therefore the WKBJ quantisation conditions take the form:

$$\frac{\alpha}{\mathrm{i}}\oint_{l_0'} q^{1/2}\,\mathrm{d}\xi = (2m+1)\pi$$
$$-\frac{\alpha}{\mathrm{i}}\oint_{l_0''} q^{1/2}\,\mathrm{d}\xi = (2n+1)\pi \qquad m, n = 0, 1, \ldots \tag{38}$$

i.e. the energy is quantised independently in each well. The necessary conditions for the approximations (38) to be valid are similar to those for the one-well case (see appendix 4), i.e.

$$\left|-\frac{\alpha}{\mathrm{i}}\oint_{l_0}(q_1-1)\,\mathrm{d}\xi\right| \ll 1 \qquad l_0 = l_0', l_0''. \tag{39}$$

On the other hand, as follows from (36), both the conditions (38) obviously fail for those energy levels for which $\exp[2S_0(b, c)]$ becomes close to unity, i.e. for a narrow potential barrier. This conclusion must be in agreement with (39). That this is the case can be easily seen by noticing that for the narrow barrier the points B and C are close each other. Therefore the integration paths both in $\tilde{\psi}^0_{2\to\bar{4}}$ and in the condition (39) have to lie near the points B and C crossing the x axis between them. The points B and C, however are singular for the integrands present in $\tilde{\psi}^0_{2\to 4}$ as well as in (39). Therefore the corresponding integrals cannot be small.

4.3.2. $k = 1$. The corresponding SG is shown in figure 8 (where we have dropped all the cut lines). It is seen from the figure that the quantisation procedure can be performed similarly to the previous case ($k = 0$). We need only replace the function $q_0(x)(\equiv q(x))$ by $(qq_1)(x)$ and to change the sub(super)script '0' into '1' in the remaining quantities appearing in the formulae (36) and (37).

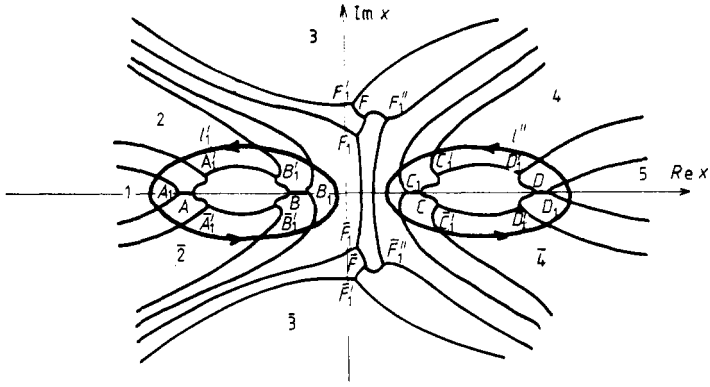

Figure 8. The first SG for the double-well potential.

Identical changes should be made also in (38) and (39) in order to get the corresponding approximate quantisation conditions as well as the conditions of their validity in the considered case. It should also be clear that the conclusions of the previous discussion of the role of the potential barrier width still remain valid.

4.3.3. Arbitrary k. The Stokes' graph for the case is shown in figure 9 (where for clarity all the cut lines are dropped). This case presents little new for the quantisation procedure in comparison with the particular cases considered earlier (except the growing complexity of the figure). This is valid for the exact quantisation as well as for its approximation. Therefore to get both the exact and the approximate formulae one should substitute in (36) and (38) q_0 by $qq_1 \ldots q_k$ and the sub(super)script '0' by 'k'. On the other hand, condition (39) becomes

$$\left| \alpha \oint_{l_k} (q_{k+1} - 1)(qq_1 \ldots q_k)^{1/2} \, \mathrm{d}\xi \right| \ll 1 \qquad l_k = l_k', l_k'' \tag{40}$$

with the paths l_k shown in figure 9.

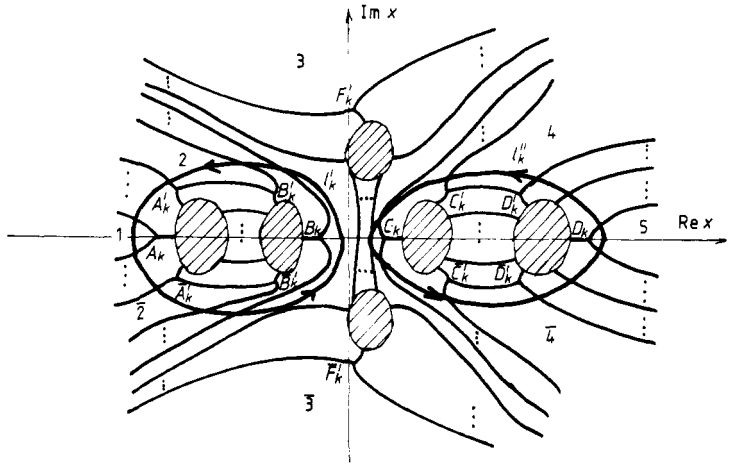

Figure 9. The kth SG for the double-well potential.

4.3.4. General case. For the sake of simplicity but without losing generality we shall consider as a general case the one having four real (but different) turning points and an arbitrary (but finite) number of complex ones. It is therefore the case of an arbitrary polynomial with many wells of which only the two deepest ones are cut by the energy level E. Having the experience of the previous cases we can consider directly the case of an arbitrary k. Figure 10 shows the corresponding SG (with the cut lines dropped). It is clear that the kth GBS conditions look as follows:

$$\frac{\alpha}{\mathrm{i}}\oint_{l_k'}(qq_1\ldots q_k)^{1/2}(x)\,\mathrm{d}x=(2m+1)\pi$$

$$-\frac{\alpha}{\mathrm{i}}\oint_{l_k''}(qq_1\ldots q_k)^{1/2}(x)\,\mathrm{d}x=(2n+1)\pi \qquad m,n=0,1,\ldots \tag{41}$$

and the conditions for their validity have the form (40) (see appendix 4). The potential barrier width plays the same role as before: the rules (41) cannot be used for the narrow barriers, for which $\exp[2S_k(B_k, C_k)]$ is close to unity. In such cases the condition (40) is not valid anymore. However, if both the conditions are fulfilled one can estimate the corrections to the energy levels. These estimations are performed in appendix 4.

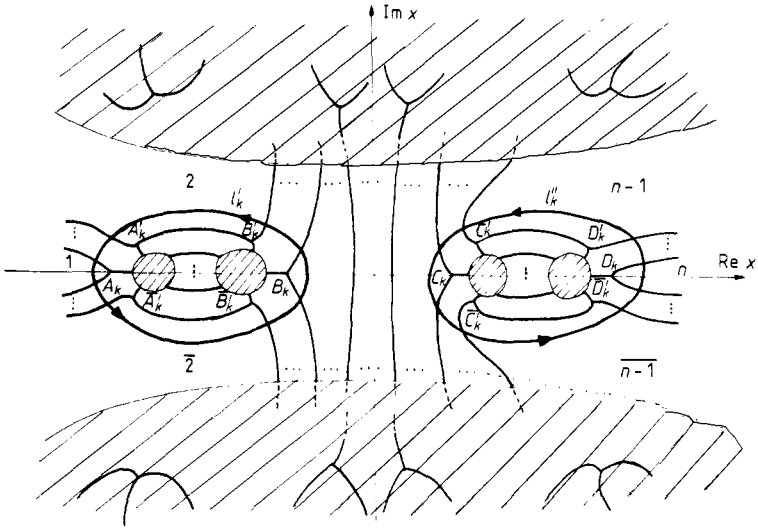

Figure 10. The kth SG for the arbitrary polynomial potential.

5. Formal asymptotic solutions to the SE and the problem of the resummation

It is natural to consider the limiting ∞th FF form of the solution to the SE. Pushing k in (15) to infinity we obtain the following, at least formal, solutions to the SE:

$$\psi_\infty^\sigma(x)=f^{-1/4}(x)\exp\left(\sigma\alpha\int_{x^0}^{x}f^{1/2}(\xi)\,\mathrm{d}\xi\right) \qquad \sigma=\pm1 \tag{42}$$

where the function f is given by

$$f(x)=\prod_{i=0}^{\infty} q_i(x_i(x)). \tag{43}$$

At first glance the ∞th FF forms (42) seem to represent the solutions to the resummation problem for the series (5) in any edition as the kth FF form ($k=0, 1, \ldots$). However, this cannot be true since in general the product (43) has to be divergent for any polynomial potential except the trivial one, $U(x)\equiv$ constant. This last statement can be justified as follows. If the function f really existed it should be the same for any sector of SG (which should also approach their definite limit for $k\to\infty$). Therefore in the limiting case $k\to\infty$ there should be only two independent solutions (42) instead of as many as the number of different sectors of the ∞th SG. On the other hand, the solutions (42) correspond strictly to the common asymptotic solutions to the SE (of which the number of independent ones is also two). Therefore the solutions (42) can be regarded merely as asymptotic in the following sense.

Let $f_k(x)$, $k=0, 1, \ldots$, denote the product of the first k factors in (43) and let $\psi_\sigma(x)$ be one of the exact solutions (15). Then we have, of course, for the appropriate sector D^σ of the Stokes' graph (see (16) and (17)):

$$\chi_k^\sigma(x)=f_k^{-1/4}(x)\exp\left(\sigma\alpha\int_{x^0}^{x} f_k^{1/2}(\xi)\,\mathrm{d}\xi\right) \tag{44}$$

$$\lim_{\alpha\to\infty}[\psi_\sigma(x)/\chi_k^\sigma(x)-1]\alpha^{2k}=0$$

$$\lim_{x\to\infty_{D^\sigma}}[\psi_\sigma(x)/\chi_k^\sigma(x)-1]=0$$

where ∞_{D^σ} is the infinity point in the sector D^σ.

Let us note however that the given kth FF forms can be regarded as the partly solved resummation problem for all the lower FF forms. It follows from (15) that between the series (5) having kth and the lth FF forms (with $k>l$) there is the relation

$$\tilde\psi_l^\sigma(x_l(x))=\exp\left(-\sigma\alpha\int_{x_l^0}^{x_k^0}(qq_1\ldots q_l)^{1/2}\,\mathrm{d}\xi\right)[q_{l+1}(x_{l+1}(x))\ldots q_k(x_k(x))]^{-1/4}$$

$$\times\exp\left(\sigma\alpha\int_{x_l^0}^{x}(qq_1\ldots q_l)^{1/2}[(q_{l+1}\ldots q_k)^{1/2}-1]\,\mathrm{d}\xi\right)\tilde\psi_k^\sigma(x_k(x)). \tag{45}$$

Since the series for $\tilde\psi_k^\sigma$ starts from a higher power of α^{-1} (i.e. from α^{-2k-1}; see appendix 2) than the series for $\tilde\psi_l^\sigma$, the relation (45) represents a kind of resummation performed with the latter series. However, since both the series (5) for $\tilde\psi_l^\sigma$ and for $\tilde\psi_k^\sigma$ are not power series in any variable it is impossible to set up the one-to-one correspondence between the terms of the series appearing on both sides of (45). Therefore it is completely obscure in what way the terms of the series for $\tilde\psi_l^\sigma$ sum to get the coefficient standing in front of $\tilde\psi_k^\sigma$ in (45). This 'hidden' resummation makes any comparison with other more standard resummation techniques difficult (see, for example, Whittaker and Watson 1963).

Finally, it should be noticed that $f(x)$ as a function of α depends rather on α^{-2}. So, expanding formally $f^{1/2}$ into the power series in α^{-2}, we reproduce the result

obtained by Fröman (1966) by direct manipulation with the corresponding asymptotic series.

6. Conclusions

We have found the infinite sequence of the new representations for the solutions to the SE, given in the FF form. These new representations have served as a source of the corresponding sequence of the approximate solutions to the SE, generalising the well known WKBJ formula. The new approximations have the following features:

(i) they can approximate the exact solution to the SE at any point (except the singular one) with an arbitrarily fixed level of accuracy, by using the kth WKBJ formula with sufficiently high k;

(ii) their asymptotic expansions in $\hbar$ (obtained simply as the standard power expansions) coincide with those of the exact solutions to a given order in $\hbar$;

(iii) they have the form of the compact WKBJ formula, being in this way its natural generalisation.

The above properties allow us to control in a quantitative way the quantisation procedure performed with these generalised WKBJ formulae (see, for example, (34), (A4.10) and (A4.13)). In particular they provide us with the relatively simple GBS conditions (33) and (41) for the energy spectrum. In general there are no essential differences (beyond the growing complexity of SG and integrations) between applications of the usual and the kth ($k>0$) WKBJ approximations. We have demonstrated it using the examples of the quantum oscillators and the double-well potential and describing the procedure in the general case.

In particular the generalised WKBJ formulae seem to be adequate for practical calculations.

We also found the formal solution to the SE defined by (42) and (43). It has the property to generate (simply by power series expansion) the asymptotic expansion in $\hbar$, having the form found previously by Fröman (1966).

Acknowledgments

It is my pleasure to thank my colleagues Drs P Kosiński, P Maślanka and J Rembieliński for many helpful discussions.

Appendix 1

We shall show below that by our choice of $U(x)$ the behaviour of any $q_k(x_k)$, $k \geq 1$, for large x, is the following:

$$q_k(x_k) \sim 1 + O(x_k^{-2}). \tag{A1.1}$$

To see this, let us note that for large x we have

$$x_1 = \sigma\alpha \int_{x^0}^{x} q^{1/2}(\xi)\, d\xi \sim x^{n+1} \tag{A1.2}$$

since $U(x) \sim x^{2n}$.

Next, for $q_1(x_1)$, as defined by (6), we obtain

$$q_1(x_1(x)) \sim 1 + O(x^{-2n-2}). \tag{A1.3}$$

Formula (A1.1) for $k=1$ follows now from (A1.2) and (A1.3). For $k>1$ one can proceed inductively noticing that, if (A1.1) is true for $k-1$, then for large x_{k-1} we have $x_k \sim x_{k-1}$ (by (11)) and $q_k\ (x_k(x_{k-1})) = 1 + O(x_{k-1}^2)$ (also by (11) and by our inductive assumption). So equation (A1.1) is true for any $k \geq 1$.

Appendix 2

We shall show below that if $\alpha \to \infty$ we have

$$q_k(x_k) \sim 1 + O(\alpha^{-2k}). \tag{A2.1}$$

We shall prove (A2.1) by induction. For $k=1$ we have, of course, equation (6) of § 2, which we rewrite as

$$q_1(x_1) = 1 + (1/\alpha^2) f_1(x) \tag{A2.2}$$

where $f_1(x)$ is independent of α. By straightforward calculations we get

$$q_2(x_2) = 1 + (1/\alpha^4) f_2(x, 1/\alpha^2) \tag{A2.3}$$

where f_2 is explicitly given by

$$f_2(x, 1/\alpha^2) = \frac{1}{4}\left[\left(f_1'' - \frac{1}{2}\frac{q'}{q} f_1'\right)\left(1 + \frac{1}{\alpha^2} f_1\right)^{-2} - \frac{5}{4}\frac{1}{\alpha^2} f_1'^2 \left(1 + \frac{1}{\alpha^2} f_1\right)^{-3}\right] q^{-1}. \tag{A2.4}$$

The function f_2 is continuously differentiable with respect to x around the point $1/\alpha^2 = 0$. Let $q_{k-1}(x_{k-1})$ have, by hypothesis, the following form:

$$q_{k-1}(x_{k-1}) = 1 + \frac{1}{\alpha^{2(k-1)}} f_{k-1}(x, 1/\alpha^2) \tag{A2.5}$$

where f_{k-1} is differentiable continuously with respect to x around the point $1/\alpha^2 = 0$. The same straightforward calculations which lead to (A2.3) and (A2.4) now give

$$q_k(x_k) = 1 + (1/\alpha^{2k}) f_k(x, 1/\alpha^2) \tag{A2.6}$$

where f_k is given by

$$f_k = \frac{1}{4}\left[\left(f_{k-1}'' - \tfrac{1}{2} f_{k-1}' \sum_{r=0}^{k-2} \frac{f_r'}{\alpha^{2r} q_r}\right)\left(1 + \frac{1}{\alpha^{2(k-1)}} f_{k-1}\right)^{-2} - \frac{5}{4}\frac{f_{k-1}'^2}{\alpha^{2(k-1)}}\left(1 + \frac{1}{\alpha^{2(k-1)}} f_{k-1}\right)^{-3}\right]\left(\prod_{r=0}^{k-2} [1 + (1/\alpha^{2r}) f_r]\right)^{-1} \tag{A2.7}$$

where $f_0 = q - 1$ and $q_0 = q$. Of course, (A2.6) proves (A2.1).

Appendix 3

We continue here the quantisation procedure for the double-well potential of § 4. The analytic continuation of ψ_{01} from sector 1 to 5 can be performed by the chain of the following equalities:

$$\begin{aligned} \psi_{01} &= \alpha^0_{1/2 \to \bar{2}} \psi_{02} + \bar{\alpha}^0_{1/2 \to \bar{2}} \psi_{0\bar{2}} \\ \psi_{02} &= \alpha^0_{2/4 \to \bar{4}} \psi_{04} + \alpha^0_{2/\bar{4} \to 4} \psi_{0\bar{4}} \\ \psi_{04} &= \alpha^0_{4/\bar{4} \to 5} \psi_{0\bar{4}} + \alpha^0_{4/5 \to \bar{4}} \psi_{05} \end{aligned} \tag{A3.1}$$

with $\alpha^0_{i/j\to k}=\lim_{x\to\infty_k}[\psi_{0i}(x)/\psi_{0j}(x)]$, where ∞_k is the infinity point in the sector k. In (A3.1) we made use of the relations $\psi_{0\bar{k}}(x)=\bar{\psi}_{0k}(\bar{x})$ for $k=2,4$.

Combining equations (A3.1) we get

$$\psi_{01}=\alpha^0\psi_{0\bar{4}}+\beta^0\psi_{05} \tag{A3.2}$$

where

$$\begin{aligned}\alpha^0&=(\alpha^0_{1/2\to\bar{2}}\alpha^0_{2/4\to\bar{4}}+\bar{\alpha}^0_{1/2\to\bar{2}}\bar{\alpha}^0_{2/4\to\bar{4}})\alpha^0_{4/\bar{4}\to 5}+\overline{(\alpha^0_{1/2\to\bar{2}}\alpha^0_{2/4\to\bar{4}}+\alpha^0_{1/2\to\bar{2}}\alpha^0_{2/4\to\bar{4}})}\\ \beta^0&=(\alpha^0_{1/2\to\bar{2}}\alpha^0_{2/4\to\bar{4}}+\bar{\alpha}^0_{1/2\to\bar{2}}\bar{\alpha}^0_{2/\bar{4}\to 4})\alpha^0_{4/5\to\bar{4}}.\end{aligned} \tag{A3.3}$$

The quantisation condition therefore becomes

$$\alpha^0=0. \tag{A3.4}$$

It needs a little effort to make (A3.4) readable. Namely, let us assume for the ψ_{0p} the following representations (cf equations (3) and (4)):

$$\begin{aligned}\psi_{01}(x)&=q_0^{-1/4}\exp[S_0(a,x)]\tilde{\psi}_{01}\\ \psi_{02}(x)&=q_0^{-1/4}\exp[-S_0(a,x)]\tilde{\psi}_{02}\\ \psi_{04}(x)&=q_0^{-1/4}\exp[S_0(d,x)]\tilde{\psi}_{04}\\ \psi_{05}(x)&=q_0^{-1/4}\exp[-S_0(d,x)]\tilde{\psi}_{05}\end{aligned} \tag{A3.5}$$

where $q_0\equiv q$, $S_0\equiv S$ and $\psi_{0p}(x)$, $p=1,2,\bar{2},4,\bar{4},5$, are given by (5). Using (A3.5) we can calculate $\alpha^0_{i/j\to k}$ in (A3.3) as follows:

$$\begin{aligned}\alpha^0_{1/2\to\bar{2}}&=-\mathrm{i}\gamma^0_{1/2\to\bar{2}}\\ \alpha^0_{2/4\to\bar{4}}&=-\mathrm{i}\exp\left(\tfrac{1}{2}\alpha\oint_{l_0'}q^{1/2}\,\mathrm{d}\xi-\tfrac{1}{2}\alpha\oint_{l_0''}q^{1/2}\,\mathrm{d}\xi-S_0(b,c)\right)\gamma^0_{2/4\to\bar{4}}\\ \alpha^0_{4/\bar{4}\to 5}&=\gamma^0_{4/\bar{4}\to 5}\\ \alpha^0_{2/\bar{4}\to 4}&=-\mathrm{i}\exp\left(\tfrac{1}{2}\alpha\oint_{l_0'}q^{1/2}\,\mathrm{d}\xi+\tfrac{1}{2}\alpha\oint_{l_0''}q^{1/2}\,\mathrm{d}\xi-S_0(b,c)\right)\gamma^0_{2/\bar{4}\to 4}\end{aligned} \tag{A3.6}$$

where $\gamma^0_{i/j\to k}=\tilde{\psi}^0_{i\to k}/\tilde{\psi}^0_{j\to k}$ (with $\tilde{\psi}^0_{i\to k}\equiv\tilde{\psi}_{0i}\ (\infty_k)$, etc) and the integration paths l_0', l_0'' are shown in figure 7. Performing further calculations we need to take into account the following general relations:

$$\tilde{\psi}^0_{i\to k}\equiv\tilde{\psi}^0_{k\to i} \tag{A3.7}$$

valid for any two sectors i, k of the SG communicated by the analytic continuation of $\tilde{\psi}_{0i}$ (or $\tilde{\psi}_{0k}$). However, for the case just considered we have additionally

$$\begin{aligned}&\tilde{\psi}^0_{1\to 2}=\tilde{\psi}^0_{4\to 5}=1\\ &\tilde{\psi}^0_{2\to\bar{2}}=\bar{\tilde{\psi}}^0_{2\to\bar{2}}\qquad\qquad\tilde{\psi}^0_{4\to\bar{4}}=\bar{\tilde{\psi}}^0_{4\to\bar{4}}.\end{aligned} \tag{A3.8}$$

Therefore if we put $\tilde{\psi}_{k\to j}=|\tilde{\psi}^0_{k\to j}|\exp(\mathrm{i}\delta^0_{k\to j})$ we get from (A3.7) and (A3.8):

$$\begin{aligned}&\delta^0_{k\to j}=\delta^0_{j\to k}\\ &\delta^0_{1\to 2}=\delta^0_{4\to 5}=\delta^0_{2\to\bar{2}}=\delta^0_{4\to\bar{4}}=0.\end{aligned} \tag{A3.9}$$

With the help of (A3.5)-(A3.9), the condition (A3.4) can be written as

$$\cos\alpha^0_+=-|\tilde{\psi}^0_{2\to\bar{4}}/\tilde{\psi}^0_{2\to 4}|\cos\alpha_- \tag{A3.10}$$

where

$$\alpha_+^0 = \frac{\alpha}{2i}\left(\oint_{l_0'} + \oint_{l_0''}\right) q_0^{1/2}\,d\xi + \delta_{2\to 4}^0$$
$$\alpha_-^0 = \frac{\alpha}{2i}\left(\oint_{l_0'} - \oint_{l_0''}\right) q_0^{1/2}\,d\xi + \delta_{2\to\bar{4}}^0. \tag{A3.11}$$

The condition (A3.10) can be still further clarified if we note that $\alpha_{i/j\to k}^0$ with $i, j, k \in (2, \bar{2}, 4, \bar{4})$ cannot all be independent. In fact we have the following relation for them, specific for the case:

$$\alpha_{4/\bar{2}\to 2}^0 = \alpha_{4/\bar{2}\to\bar{4}}^0/(1-|\alpha_{\bar{4}/4\to 2}|^2) \tag{A3.12a}$$

or in terms of ψ

$$|\tilde{\psi}_{2\to\bar{4}}^0/\tilde{\psi}_{2\to 4}^0|^2 = 1 + (\tilde{\psi}_{4\to\bar{4}}^0\tilde{\psi}_{2\to\bar{2}}^0/|\tilde{\psi}_{2\to 4}^0|^2)\exp[2S_0(b, c)]. \tag{A3.12b}$$

Equations (A3.12) can be easily obtained by considering the linear dependence between the solutions ψ_{0k}, with $k = 2, \bar{2}, 4, \bar{4}$.

Substituting (A3.12) into (A3.10) we finally get the quantisation condition (A3.4) in the form given by (36).

Appendix 4

We discuss here the conditions (28), (30), (39) and (40) and also estimate the corrections to the energy levels obtained with the help of the GBS quantisation conditions. Both the conditions and the corrections can be justified by using the exact solutions (15) in the quantisation procedure instead of their approximations (17). Let us do this first for the one-well case. If we do that the quantisation condition (33) should be replaced by

$$-\frac{\alpha}{i}\oint_{l_k}(qq_1\ldots q_k)^{1/2}\,d\xi + 2\delta_k = (2n+1)\pi \tag{A4.1}$$

where the additional phase δ_k in (A4.1) is defined by

$$\exp(2i\delta_k) = \tilde{\psi}_k^\sigma(x_k(\infty_3))/\overline{\tilde{\psi}_k^\sigma(x_k(\infty_3))} \tag{A4.2}$$

with $\tilde{\psi}_k^\sigma(x_k(x))$ given by (15) and (5) and ∞_3 being the infinity point in sector 3 of figure 6. It follows from (A4.2) and (5) that δ_k is negligible in (A4.1) if

$$\inf\left(\alpha\int_\gamma |q_{k+1}-1||qq_1\ldots q_k|^{1/2}|d\xi|\right) \ll 1 \tag{A4.3}$$

where the paths γ are shown in figure 6. Indeed, let us write $\tilde{\psi}_k^\sigma(x_k(\infty_3))$ as $1+a$ and let b and b' denote the values of the LHS of (A4.3) and (34), respectively. Then, by simple estimations, we have

$$|a| < b\,e^b \qquad b' < 2b. \tag{A4.4}$$

On the other hand, for the phase δ_k we have

$$2i\delta_k = \ln(1+a) - \ln(1+\bar{a}) = \sum_{n\geq 1}\frac{(-1)^{n+1}}{n}(a^n - \bar{a}^n). \tag{A4.5}$$

From (A4.5) it now follows that

$$|\delta_k| < |a|/(1-|a|) < 2|a| \tag{A4.6}$$

if $|a| < \frac{1}{2}$.

Therefore the condition (34) is at least necessary, if the quantisation condition (33) is to be satisfied.

Let us note further that if (A4.3) is fulfilled then we can even estimate the value of δ_k, since in such a case the RHS of (A4.5) can be approximated by

$$\alpha\left(\int_\gamma - \int_{\bar\gamma}\right)(q_{k+1}-1)(qq_1 \dots q_k)^{1/2}\,\mathrm{d}\xi = -\alpha \oint_{l_k} (q_{k+1}-1)(qq_1 \dots q_k)^{1/2}\,\mathrm{d}\xi \tag{A4.7}$$

where $\bar\gamma$ is the path complex conjugate to γ. Therefore for δ_k we get

$$2\delta_k \approx -\frac{\alpha}{\mathrm{i}} \oint_{l_k} (q_{k+1}-1)(qq_1 \dots q_k)^{1/2}\,\mathrm{d}\xi. \tag{A4.8}$$

Having estimated δ_k it is possible to find the corrections to the energy E_m calculated with the help of the GBS conditions (33). Namely, subtracting (33) from (A4.1) we get

$$\Delta\alpha_m = -2\delta_k \left[\frac{\mathrm{d}}{\mathrm{d}\alpha}\left(-\frac{\alpha}{\mathrm{i}} \oint_{l_k} (qq_1 \dots q_k)^{1/2}\,\mathrm{d}\xi\right)\right]^{-1}\Bigg|_{\alpha=\alpha_m}. \tag{A4.9}$$

Substituting (A4.8) in (A4.9) we obtain finally

$$\begin{aligned}\frac{\Delta E_m}{E_m} &= 2\frac{n}{n+1}\frac{\Delta\alpha_m}{\alpha_m} \\ &= -2\frac{n}{n+1}\left\{\oint_{l_k} (q_{k+1}-1)(qq_1 \dots q_k)^{1/2}\,\mathrm{d}\xi \right. \\ &\quad \left. \times\left[\frac{\mathrm{d}}{\mathrm{d}\alpha}\left(\alpha \oint_{l_k} (qq_1 \dots q_k)^{1/2}\,\mathrm{d}\xi\right)\right]^{-1}\right\}_{\alpha=\alpha_m}\end{aligned} \tag{A4.10}$$

where $2n$ is the degree of the polynomial potential $U(x)$.

Let us consider further the double-well case. It is seen from (36) that the conditions for (38) to be valid are

$$\begin{aligned}&|\rho^k \exp[2S_k(b,c)]| \ll 1 \\ &|\delta^k_{2\to 4} + \delta^k_{2\to\bar 4}| \ll 1 \\ &|\delta^k_{2\to 4} - \delta^k_{2\to\bar 4}| \ll 1.\end{aligned} \tag{A4.11}$$

The last two inequalities mean that both the phases $\delta_{2\to 4}$ and $\delta_{2\to\bar 4}$ have to be small. One can therefore reason in the same way as before to obtain the following estimates for the phases:

$$\begin{aligned}\delta^k_{2\to 4} + \delta^k_{2\to\bar 4} &\approx -\frac{\alpha}{\mathrm{i}} \oint_{l'_k} (q_{k+1}-1)(qq_1 \dots q_k)^{1/2}\,\mathrm{d}\xi \\ \delta^k_{2\to 4} - \delta^k_{2\to\bar 4} &\approx \frac{\alpha}{\mathrm{i}} \oint_{l''_k} (q_{k+1}-1)(qq_1 \dots q_k)^{1/2}\,\mathrm{d}\xi.\end{aligned} \tag{A4.12}$$

Following the previous procedure to estimate the energy corrections and using (36), (38) and (A4.12) we get for the left well

$$\frac{\Delta E'_m}{E'_m} = 2\frac{n}{n+1}\left\{\alpha^{-1}\rho^k \exp[2S_k(b_k, c_k)]\left[1+\exp\left(-\alpha\oint_{l''_k}(qq_1\ldots q_k)^{1/2}\,d\xi\right)\right]^{-1}\right.$$
$$\left.-\oint_{l'_k}(q_{k+1}-1)(qq_1\ldots q_k)^{1/2}\,d\xi\right\}$$
$$\times\left[\frac{d}{d\alpha}\left(-\alpha\oint_{l'_k}(qq_1\ldots q_k)^{1/2}\,d\xi\right)\right]^{-1}\Bigg|_{\alpha=\alpha_m} \qquad \text{(A4.13)}$$

with the completely analogous expression for the right well. Let us note that in principle we cannot drop the exponential term in (A4.13). It can be as large as the second one. It should be realised that the corrections (A4.13) do not apply to the energy levels calculated by asymptotic expansion in $\hbar$. Therefore the exponential term in (A4.13) cannot be regarded as exponentially small and consequently as subdominant (see, for example, Balian *et al* (1979) for the relevant discussion).

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