IOPscience iopscience.iop.org

Home Search Collections Journals About Contact us My IOPscience

Error bounds for the Bohr - Sommerfeld formula

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1996 J. Phys. A: Math. Gen. 29 7229

(http://iopscience.iop.org/0305-4470/29/22/020)

View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 171.66.16.70
The article was downloaded on 02/06/2010 at 04:04

Please note that terms and conditions apply.

J. Phys. A: Math. Gen. **29** (1996) 7229–7257. Printed in the UK

Error bounds for the Bohr–Sommerfeld formula

L V Chebotarev
Case Postale 655, Montreal, Quebec, Canada, H2A 3N2

Received 29 May 1996

Abstract. Exact error bounds to the Bohr–Sommerfeld quantization formula are derived without *a priori* assuming quantum numbers to be large. The assessments are expressed in terms of a *single* quantity, the error-control integral, which is determined by the potential $U(x)$ in a unique fashion as a function of a particle's total energy. While taken over the real axis, the integral has the advantage of being suitable for analytical investigation. Exact sufficient conditions are established for the Bohr–Sommerfeld formula to be extendible to the range of lower quantum numbers.

1. Introduction

The Bohr–Sommerfeld quantization formula is widely used in physics. Its significance is not limited to the specific problem for which it was originally derived, namely, that of determining the energy levels of a particle in a potential well. The formula plays an essential role in the foundations of the theory of quantum fields, solitons, and instantons [1]. It is used in the theory of chemical reactions [2] for evaluating resonance phase shifts in molecular orbiting collisions. This quantization formula provides a starting point for the derivation of the Onsager–Lifshitz relations, which play the key role in the theory of magneto-oscillatory phenomena in metals at low temperatures [3]. In quantum mechanics, new approaches to specific problems are based on the Bohr–Sommerfeld formula [4].

The importance of the Bohr–Sommerfeld formula appears in a new light due to recent advances in nanotechnologies [5], which have given rise to a general increase of interest in quantum processes occurring at nanoscales. New designs are needed to ensure the reliable functioning of all components of nanodevices at such dimensions, when quantum features of electron motion come to be essential. That is why the need for better fundamental understanding of quantum transport phenomena has become urgent [6, 7]. However, a reliable kinetic theory, which is applicable to the nanometer regime, may be developed only on the basis of an accurate mathematical description of basic quantum effects. In view of the fact that exact solutions are not possible except for a few simplest cases, the need for approximate methods with controlled accuracy is now clearly realized [4, 7].

According to a widely accepted point of view, the Bohr–Sommerfeld quantization formula is valid only for large quantum numbers $n \gg 1$. Really, rigorous mathematical theorems [8–10] have established the fact that the error term δ_n, by which the Bohr–Sommerfeld formula differs from an exact equation, vanishes as $n \to \infty$. It should be noted, however, that those theorems are based on an essential premise that the potential $U(x)$ increases *unboundedly* as $|x| \to \infty$. Besides, those theorems result only in relations that are asymptotic in their nature, i.e. they establish the proof for δ_n to be some kind of O-term as $n \to \infty$. The theorems provide no indication as to the error bounds for δ_n.

0305-4470/96/227229+29$19.50 © 1996 IOP Publishing Ltd

It was, however, noticed long ago that the actual accuracy of the Bohr–Sommerfeld formula is much higher than one would expect in view of the restrictions due to the method used for its derivation. There are many indications that, in fact, this formula might be extended, under certain conditions, to the range of lower quantum numbers n. Indeed, as is well known, in some problems (hydrogen atom, harmonic oscillator) the Bohr–Sommerfeld formula yields exact results for all positive integers n, starting with the smallest ones. In many other problems, numerical investigation shows the relative errors associated with the Bohr–Sommerfeld formula to be surprisingly small even for $n \sim 1$. Thus, for instance, numerical evaluations [11, 12] of energy levels of an anharmonic oscillator, which is described by a potential $U(x) = \omega^2 x^2 + \lambda x^4$, showed that even in the strong-coupling limit ($\lambda \gg \omega^2$), the values produced by the Bohr–Sommerfeld formula are incorrect by 1% or less for all levels except for the ground state which is off by about 22%.

The first proof for the fact that the Bohr–Sommerfeld formula is applicable, under certain conditions, to the lower energy levels was given by Birkhoff [13]. An independent derivation of Birkhoff's assessments was made by Kemble [14, 15] within the framework of the phase-integral method. According to calculations performed by Kemble [14] for the normal state of the H_2 molecule, described by the Morse potential, the Bohr–Sommerfeld formula yields the energy value that is correct to one-third of a per cent of the spacing of adjacent energy levels. Further developments of this method were discussed in references [2, 10, 16, 17].

The assessments of the error bounds to the Bohr–Sommerfeld formula, as obtained by the phase-integral method, necessitate a search for optimal paths in the complex plane which provide minimum values to certain integrals of rather complicated functions. This cannot be done without taking into account the detailed analytic structure of the potential $U(x)$ which is often found to be rather complicated. For this reason, the assessments of that kind, while suitable for numerical evaluations with respect to a given particular potential, are difficult to use when one is interested in analytical investigation. Indeed, the question of particular interest is most often not that about a number. The problem resides rather in establishing sufficient conditions, formulated in terms of parameters associated with the potential $U(x)$, for the error terms to be negligible. Besides, application of the phase-integral method is restricted only to potentials that admit of analytic continuation from the real axis into the complex plane. In view of the importance of the problem, and its complexity, a satisfactory solution may be found only by combining different approaches, thus putting to use the advantages of every one of them.

Some useful information on the accuracy of the Bohr–Sommerfeld formula may also be obtained by investigating higher-order correction terms as obtained within the phase-integral method [12, 18]. However, the first terms of an infinite series do not always provide the right impression about the behaviour of the series as a whole. A reliable assessment for the sum of the series as a whole is needed in general. The problem is too complicated to expect simple solutions.

The phase-integral method is not the only possible way of obtaining proper assessments. In reality, it is not so difficult to derive an upper bound to the error terms related to the Bohr–Sommerfeld formula. The fact is that an estimated upper bound to the error is *inevitably* found to be greater than the actual error. This feature is inherent in the very nature of such estimations. The main problem thus consists not so much in deriving *any kind* of upper bound, but rather in obtaining the *lowest possible* upper bound to the error terms involved with the use of the Bohr–Sommerfeld formula. Advances in the theory of asymptotic solution of linear differential equations of the second order [10, 19] provide appropriate means for handling the problem. In the fundamental work by Olver [19], a rigorous proof

was obtained for the fact that, under certain conditions, the Bohr–Sommerfeld formula is valid *uniformly* with respect to all non-negative integer values of the quantum number $n \in [0, n_m]$, provided the Schrödinger equation contains a large (unspecified) parameter u, where $n_m \sim u \gg 1$ (consider the last paragraph of section 6.4 on p 162 along with the formula (2.5) in [19]). However, final results were written in [19] only as asymptotic relations. Explicit error bounds for the correction terms have not been obtained.

In the present paper, the assessments of the error terms associated with the Bohr–Sommerfeld formula are derived without any *a priori* restriction upon the quantum numbers n. The derivation is based on Olver's theory [10, 19]. This method is known to produce the best results as to establishing the lowest possible upper bounds for the correction terms in asymptotic expansions. The final assessment (4.100) obtained below for the error term to the Bohr–Sommerfeld formula is expressed in terms of the *error-control integral* $\mathrm{E}(n)$ (3.89), which is taken *over the real axis* and depends on a real, continuous, and strictly increasing function $\xi = \xi(x)$ (equations (3.50*a–c*). The function $\xi(x)$ is completely determined by the potential $U(x)$. It defines a one-to-one mapping of the real x axis onto the corresponding ξ axis. This mapping, and its properties, make the point of the ensuing analysis.

The integral $\mathrm{E}(n)$ is found to be well suited for analytical investigations of sufficient conditions for the Bohr–Sommerfeld formula to be extended to the range of lower quantum numbers. Due to the scaling symmetry of the expression (3.89), the properties of $\mathrm{E}(n)$, as a function of parameters associated with the potential $U(x)$, may easily be established. Furthermore, modern computing facilities make the evaluation of remaining numbers of the order of unity not too difficult.

In section 2, fundamental solutions of the Weber equation are specified and related auxiliary functions are investigated. Our approach to an approximate solution of the bound-state problem is discussed in section 3. The exact equation for the energies of the bound states is written in section 4, along with sufficient conditions under which this equation reduces to the Bohr–Sommerfeld quantization formula. A comparison with the known exact solution of the bound-state problem for the finite-range potential $U(x) = -|U_0|/\cosh^2(x/l)$ is made in section 5. Connection to the WKB approximation is discussed in section 6. Conclusions and comparison with reference [19] are given in section 7. Throughout the paper we use units with $\hbar = 1$.

2. Fundamental solutions of the Weber equation

2.1. Specification of fundamental solutions

Let us consider the Weber equation

$$\frac{\mathrm{d}^2 w}{\mathrm{d}x^2} + (\nu + \tfrac{1}{2} - \tfrac{1}{4}x^2)w = 0 \tag{2.1}$$

on the real axis $x \in (-\infty, +\infty)$, with a real parameter $\nu > -1/2$. As a fundamental pair of solutions to equation (2.1) we take the functions $w_\nu(x)$ and $u_\nu(x)$ defined by

$$w_\nu(x) = \left(\frac{\pi}{2}\right)^{1/4} \Gamma^{-1/2}(\nu+1) D_\nu(x) \tag{2.2}$$

$$u_\nu(x) = \frac{\Gamma^{1/2}(\nu+1)}{2^{3/4}\pi^{1/4}} [\mathrm{e}^{-\mathrm{i}\pi(\nu+1)/2} D_{-\nu-1}(-\mathrm{i}x) + \mathrm{e}^{\mathrm{i}\pi(\nu+1)/2} D_{-\nu-1}(\mathrm{i}x)] \tag{2.3}$$

where $\Gamma(z)$ is the gamma function and $D_\nu(z)$ is the standard designation for the parabolic cylinder functions [20, p 323]. In this section we give a summary of important properties of the functions $w_\nu(x)$ and $u_\nu(x)$ that are essential for subsequent proofs. All the following

relations are obtainable from the known properties of the parabolic cylinder functions [20, ch VIII].

The Wronskian of the functions $w_\nu(x)$ and $u_\nu(x)$

$$W\{w_\nu(x), u_\nu(x)\} = w_\nu(x)u'_\nu(x) - u_\nu(x)w'_\nu(x) = 1 \tag{2.4}$$

is identically equal to unity so the functions (2.2) are linearly independent for all $\nu > -1/2$.

The connection formulae for the functions $w_\nu(x)$ and $u_\nu(x)$ reduce to simple relations. For every $\nu > -1/2$ and any real $x \in (-\infty, +\infty)$ we find

$$\begin{aligned} w_\nu(-|x|) &= w_\nu(|x|)\cos\pi\nu - u_\nu(|x|)\sin\pi\nu \\ u_\nu(-|x|) &= -w_\nu(|x|)\sin\pi\nu - u_\nu(|x|)\cos\pi\nu. \end{aligned} \tag{2.5}$$

The Taylor series expansions for the functions $w_\nu(x)$ and $u_\nu(x)$,

$$\begin{aligned} w_\nu(x) &= \frac{2^{\nu/2}\Gamma^{-1/2}(\nu+1)}{(2\pi)^{1/4}}\mathrm{e}^{x^2/4}\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\left(x\sqrt{2}\right)^n\Gamma\left(\frac{1+n+\nu}{2}\right)\cos\left[\frac{\pi(\nu+n)}{2}\right] \\ u_\nu(x) &= -\frac{2^{\nu/2}\Gamma^{-1/2}(\nu+1)}{(2\pi)^{1/4}}\mathrm{e}^{x^2/4}\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\left(x\sqrt{2}\right)^n\Gamma\left(\frac{1+n+\nu}{2}\right)\sin\left[\frac{\pi(\nu+n)}{2}\right] \end{aligned} \tag{2.6}$$

are convergent for all finite x.

For any fixed $\nu > -1/2$, the function $w_\nu(x)$ exponentially decreases, whereas the function $u_\nu(x)$ exponentially increases as $x \to +\infty$.

$$\begin{aligned} w_\nu(x) &\sim \left(\frac{\pi}{2}\right)^{1/4}\Gamma^{-1/2}(\nu+1)\mathrm{e}^{-x^2/4}x^\nu \qquad (x \to +\infty) \\ u_\nu(x) &\sim \left(\frac{2}{\pi}\right)^{1/4}\Gamma^{1/2}(\nu+1)\mathrm{e}^{x^2/4}x^{-\nu-1} \qquad (x \to +\infty). \end{aligned} \tag{2.7}$$

On the other hand, uniform asymptotic representations for the functions $w_\nu(x)$ and $u_\nu(x)$, for large ν, are found to be

$$\begin{aligned} w_\nu(x) &\sim \sqrt{\pi}\left[\frac{\zeta(x)}{\frac{1}{4}x^2 - \nu - \frac{1}{2}}\right]^{1/4}\mathrm{Ai}(\zeta) \qquad (\nu \gg 1,\ x \geqslant 0) \\ u_\nu(x) &\sim \sqrt{\pi}\left[\frac{\zeta(x)}{\frac{1}{4}x^2 - \nu - \frac{1}{2}}\right]^{1/4}\mathrm{Bi}(\zeta) \qquad (\nu \gg 1,\ x \geqslant 0) \end{aligned} \tag{2.8}$$

where $\zeta = \zeta(x)$ while $\mathrm{Ai}(\zeta)$ and $\mathrm{Bi}(\zeta)$ are the Airy functions. The function $\zeta(x)$ in the expressions (2.8) is a continuous even function on the whole of the real axis. On the interval $[0, +\infty)$ (i) $\zeta(x)$ is strictly increasing, (ii) $\zeta(x)$ has a single zero at the point $x = 2\sqrt{\nu + 1/2}$, (iii) $\zeta(x)$ has a continuous derivative, (iv) $\zeta(x)$ has the values determined by

$$\begin{aligned} &\tfrac{2}{3}[-\zeta(x)]^{3/2} = \int_x^{2\sqrt{\nu+1/2}}\mathrm{d}x\left(\nu + \frac{1}{2} - \frac{x^2}{4}\right)^{1/2} \qquad 0 \leqslant x \leqslant 2(\nu+\tfrac{1}{2})^{1/2} \\ &\tfrac{2}{3}[\zeta(x)]^{3/2} = \int_{2\sqrt{\nu+1/2}}^{x}\mathrm{d}x\left(\frac{x^2}{4} - \nu - \frac{1}{2}\right)^{1/2} \qquad 2(\nu+\tfrac{1}{2})^{1/2} \leqslant x < +\infty \\ &\zeta(-x) = \zeta(x) \qquad \zeta'(-x) = -\zeta'(x) \qquad \zeta(0) = -\left[\frac{3\pi}{4}\left(\nu + \frac{1}{2}\right)\right]^{2/3}. \end{aligned} \tag{2.9}$$

The precision of the uniform asymptotic representations (2.8) is found to be remarkably high. Even for $\nu \sim 1$ the relative error associated with the asymptotic formulae (2.8) does

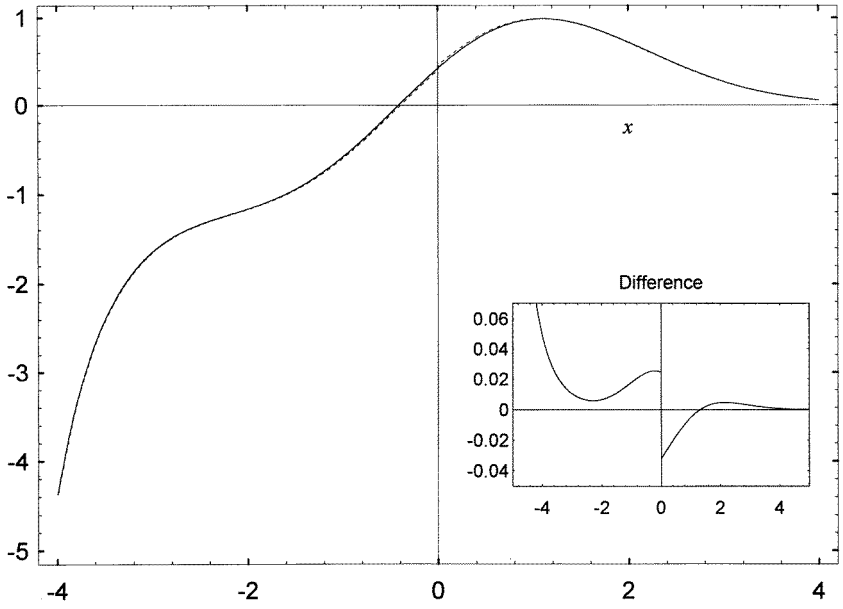

Figure 1. Function $w_\nu(x)$ (full curve) and its uniform approximation (broken curve). The approximate values have been calculated by use of the uniform asymptotic representations (2.8) along with the connection formulae (2.5). The graphs are plotted for $\nu = 0.7$. Inset: Difference between the exact values of the function $w_\nu(x)$ and its approximate values, plotted as a function of x.

not exceed a few per cent. To give an idea of the high precision of the formulae (2.8), the graph of the function $w_\nu(x)$ is plotted in figure 1 for $\nu = 0.7$ as a full curve. The broken curve in the figure represents the approximate values of $w_\nu(x)$ as obtained from (2.8) along with (2.5). The difference between the two curves is hardly discernible in figure 1 so it is also plotted in the inset to figure 1, on being appropriately scaled.

The asymptotic behaviour of the functions $w_\nu(x)$ and $u_\nu(x)$ on the negative real axis is readily derived from equations (2.7) or (2.8) by use of the connection formulae (2.5). The graphs of $w_\nu(x)$ (full curve) and $u_\nu(x)$ (broken curve), for $\nu = 4.1$, are plotted in figure 2. The approximate values of the function $w_\nu(x)$, for the same $\nu = 4.1$, have also been calculated by using the asymptotic forms (2.8) along with the connection formulae (2.5). Those approximate values are represented by the chain curve in figure 2. This latter curve is, however, not distinguishable from the full curve in figure 2 since the deviation of the exact values from the approximate ones does not exceed 6×10^{-3} in the investigated range $|x| \leqslant 6$. To make it visible, this deviation is plotted on the proper scale in the inset to figure 2 as a function of x, for $w_\nu(x)$ with $\nu = 4.1$. The figure provides still another illustration for the high precision of the asymptotic formulae (2.8). This fact is to be kept in mind when considering the real meaning of the formal condition $\nu \gg 1$, which determines the validity of the asymptotic formulae (2.8).

2.2. Auxiliary functions related to $w_\nu(x)$ and $u_\nu(x)$

2.2.1. Interval $0 \leqslant x < +\infty$. To establish the required error bounds for correction terms considered below, the assessments of the functions $w_\nu(x)$ and $u_\nu(x)$ are needed. Let us first consider the positive real axis $x \geqslant 0$. Following reference [19, section 5], for every

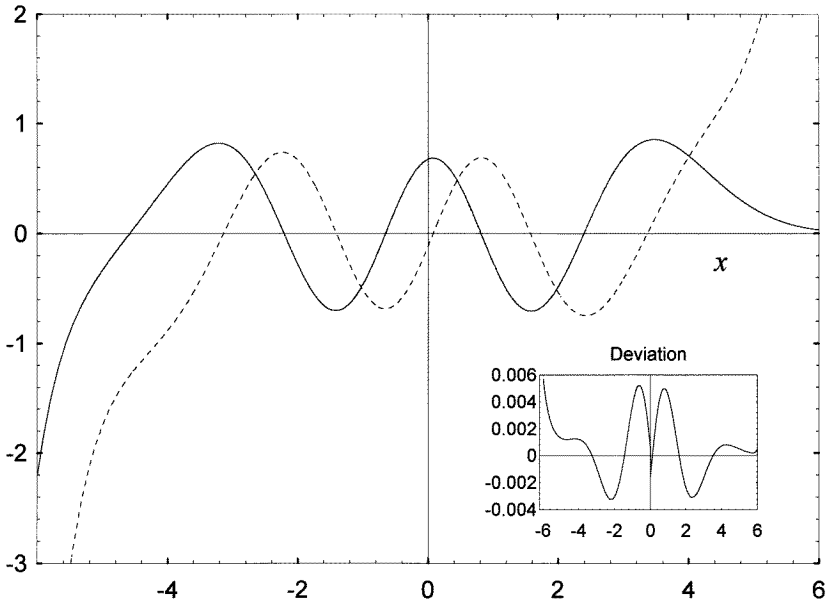

Figure 2. Functions $w_\nu(x)$ (full curve) and $u_\nu(x)$ (broken curve). The graphs are plotted for $\nu = 4.1$. Also there is a chain curve that represents approximate values of the function $w_\nu(x)$, for the same $\nu = 4.1$, which were calculated by using the asymptotic forms (2.8) along with the connection formulae (2.5). This chain curve is, however, not distinguishable from the full curve. Inset: Deviation of the exact values of the function $w_\nu(x)$ from its approximate values, plotted as a function of x.

$\nu > -1/2$ we introduce a *modulus function* $M_\nu(x)$, *phase function* $\theta_\nu(x)$, and *weight function* $E_\nu(x)$, related by

$$w_\nu(x) = \frac{M_\nu(x)}{E_\nu(x)} \cos\theta_\nu(x) \qquad u_\nu(x) = M_\nu(x) E_\nu(x) \sin\theta_\nu(x). \tag{2.10}$$

For $x \geqslant 0$, the function $E_\nu(x)$ is defined in accordance with [19, section 5]

$$\begin{aligned} &E_\nu(x) = 1 \qquad (0 \leqslant x \leqslant c_\nu) \\ &E_\nu(x) = \left[\frac{u_\nu(x)}{w_\nu(x)}\right]^{1/2} \qquad (c_\nu \leqslant x < +\infty) \end{aligned} \tag{2.11}$$

where $x = c_\nu$ is the greatest positive root of the equation (cf figure 2)

$$w_\nu(x) = u_\nu(x). \tag{2.12}$$

The parameter c_ν is a positive and monotonically increasing function of $\nu > -1/2$ (cf [19, section 5]). At $\nu = 0$, $c_0 = 1.034\,776$ (correct to six decimal places), and c_ν tends to zero as $\nu \to -1/2+$. From (2.6) we find

$$c_\nu \sim \tfrac{1}{4}\Gamma^2(\tfrac{1}{4})(\nu + \tfrac{1}{2}) \qquad (\nu \to -1/2+). \tag{2.13}$$

All the zeros of the functions $w_\nu(x)$ and $u_\nu(x)$ may be shown to lie to the left of c_ν. On the positive real axis $E_\nu(x)$ is a *non-decreasing* function of x which is not less than unity [19].

With the definition (2.11), equations (2.10) yield

$$M_\nu(x) = \begin{cases} \sqrt{w_\nu^2(x) + u_\nu^2(x)} & (0 \leqslant x \leqslant c_\nu) \\ \sqrt{2w_\nu(x)u_\nu(x)} & (c_\nu \leqslant x < +\infty) \end{cases} \tag{2.14}$$

and

$$\begin{aligned} \theta_\nu(x) &= \frac{\pi}{4} - \int_x^{c_\nu} \frac{\mathrm{d}x}{M_\nu^2(x)} \qquad (0 \leqslant x \leqslant c_\nu) \\ \theta_\nu(x) &= \frac{\pi}{4} \qquad (c_\nu \leqslant x < +\infty). \end{aligned} \tag{2.15}$$

In particular, substituting (2.6) in (2.14), we find

$$M_\nu(0) = \frac{2^{\nu/2}}{(2\pi)^{1/4}\Gamma^{1/2}(\nu+1)}\Gamma\left(\frac{1+\nu}{2}\right). \tag{2.16}$$

The asymptotic behaviour of the functions $E_\nu(x)$ and $M_\nu(x)$, with $\nu > -1/2$ being fixed while $x \to +\infty$, is obtained from (2.7)

$$E_\nu(x) \sim \left(\frac{2}{\pi}\right)^{1/4} \Gamma^{1/2}(\nu+1)\mathrm{e}^{x^2/4}x^{-(\nu+1/2)} \qquad x \to +\infty \tag{2.17}$$

$$M_\nu(x) \sim \sqrt{\frac{2}{x}} \qquad x \to +\infty. \tag{2.18}$$

On the other hand, uniform asymptotic representations for $E_\nu(x)$ and $M_\nu(x)$, as $\nu \gg 1$ and $x \geqslant 0$ being fixed, may be obtained from (2.11) and (2.14) by using (2.8). First we notice that, for $\nu \gg 1$, the root $x = c_\nu$ of equation (2.12) is asymptotically given by $c_\nu \sim x_c$, where x_c is determined from the equation (cf [10, p 395])

$$\zeta(x_c) = c = -0.366\,046 \tag{2.19}$$

with $\zeta(x)$ defined by (2.9). Thus we obtain, for $\nu \gg 1$ and $x \geqslant 0$,

$$E_\nu(x) \sim \mathrm{E}(\zeta) \tag{2.20}$$

$$M_\nu(x) \sim \sqrt{\pi}\left[\frac{\zeta(x)}{\frac{1}{4}x^2 - \nu - \frac{1}{2}}\right]^{1/4} \mathrm{M}(\zeta) \tag{2.21}$$

$$\theta_\nu(x) \sim \frac{\pi}{2} - \Theta(\zeta) \tag{2.22}$$

with $\zeta \equiv \zeta(x)$, whereas $\mathrm{E}(x)$, $\mathrm{M}(x)$, and $\Theta(x)$ are the auxiliary functions introduced in reference [10, p 394] as related to the Airy functions.

For every $\nu \geqslant -1/2$, we associate with the function $M_\nu(x)$ an important positive number σ_ν defined by

$$\sigma_\nu = \sup_{x\in[0,+\infty)}\left[\left|\frac{x^2}{4} - \nu - \frac{1}{2}\right|^{1/2} M_\nu^2(x)\right]. \tag{2.23}$$

In view of the asymptotic relation (2.18) for $M_\nu(x)$, we find for every fixed $\nu \geqslant -1/2$

$$\lim_{x\to+\infty}\left[\left|\frac{x^2}{4} - \nu - \frac{1}{2}\right|^{1/2} M_\nu^2(x)\right] = 1. \tag{2.24}$$

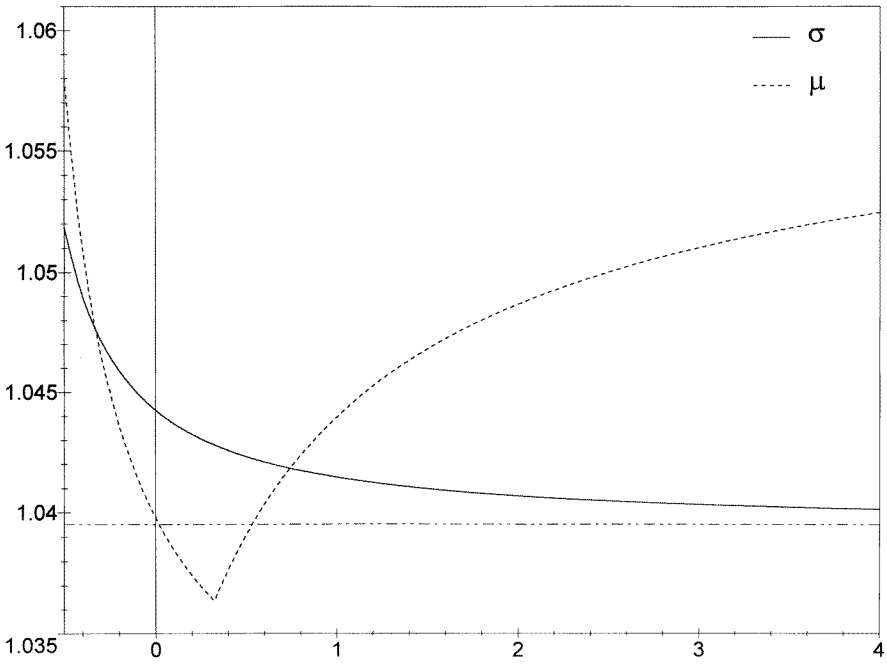

Figure 3. Parameters σ_ν (full curve) and μ_ν (broken curve) as functions of ν.

Hence the right-hand side of (2.23) is bounded in magnitude for every finite $\nu \geqslant -1/2$. On the other hand, as $\nu \to +\infty$, the limiting value of σ_ν may be found by substituting the uniform asymptotic representation (2.21) for $M_\nu(x)$ in the expression (2.23). We get

$$\lim_{\nu\to+\infty} \sigma_\nu = \sup_{\zeta\in(-\infty,+\infty)} [\pi|\zeta|^{1/2}\mathrm{M}^2(\zeta)] = \lambda = 1.039\,523 \tag{2.25}$$

where the number λ was first introduced in [10, p 397] relative to the Airy functions. The graph of σ_ν (as a function of ν) is plotted as a full curve in figure 3. We see that σ_ν is a continuous, strictly decreasing function of $\nu \in [-1/2, +\infty)$ which takes on its maximum value $\sigma_{\max} = 1.051\,839$ at $\nu = -1/2$, and that it slowly decreases with increasing ν while approaching its limiting value λ (2.25). In particular, $\sigma_0 = 1.044\,231$ at $\nu = 0$.

2.2.2. Extension to the interval $-c_\nu \leqslant x < 0$. The connection formulae (2.5) allow us to extend the relations (2.10) to the interval $[-c_\nu, 0]$. On this interval, we define the function $E_\nu(x)$ by

$$E_\nu(x) = 1 \qquad (-c_\nu \leqslant x \leqslant 0). \tag{2.26}$$

The main property of $E_\nu(x)$, namely that of being a positive, non-decreasing function which is not less than unity, is thus preserved for $x \in [-c_\nu, +\infty)$. Then the connection formulae (2.5) show $M_\nu(x)$ to be even function in the *oscillatory region* $[-c_\nu, c_\nu]$,

$$M_\nu(-x) = M_\nu(x) \qquad (-c_\nu \leqslant x \leqslant c_\nu). \tag{2.27}$$

For the phase function $\theta_\nu(x)$, the connection formulae (2.5) yield the relation

$$\theta_\nu(-|x|) = -\theta_\nu(|x|) - \pi\nu \qquad (-c_\nu \leqslant x \leqslant c_\nu). \tag{2.28}$$

Taking advantage of the identity

$$\frac{2}{\pi}\int_0^{c_\nu}\frac{\mathrm{d}x}{M_\nu^2(x)}=\nu+\tfrac{1}{2} \tag{2.29}$$

we derive from (2.28)

$$\theta_\nu(x)=\frac{\pi}{4}-\int_x^{c_\nu}\frac{\mathrm{d}x}{M_\nu^2(x)}\qquad(-c_\nu\leqslant x\leqslant c_\nu). \tag{2.30}$$

Hence $\theta_\nu(x)$ is found to be a continuous and strictly increasing function on the interval $[-c_\nu, c_\nu]$. Its total increase, when x ranges from $-c_\nu$ through c_ν, is thus equal to $\pi(\nu+1/2)$.

The expressions (2.10) cannot be extended to the left of the point $x=-c_\nu$ without loss of essential properties of the function $E_\nu(x)$. Instead, for $x\in(-\infty,-c_\nu)$, the general relations (2.5) are to be used in order to express the functions $w_\nu(x)$ and $u_\nu(x)$ in terms of $M_\nu(x)$ and $E_\nu(x)$.

2.3. Auxiliary functions related to the derivatives $w_\nu'(x)$ and $u_\nu'(x)$

Modulus and phase functions $N_\nu(x)$ and $\omega_\nu(x)$ relative to the derivatives $w_\nu'(x)$ and $u_\nu'(x)$ of the functions (2.2) and (2.3) with respect to x, are also needed for further assessments. They are defined by (cf [19, p 156])

$$w_\nu'(x)=\frac{N_\nu(x)}{E_\nu(x)}\cos\omega_\nu(x)\qquad u_\nu'(x)=N_\nu(x)E_\nu(x)\sin\omega_\nu(x) \tag{2.31}$$

with the same definitions (2.11) and (2.26) for the weight function $E_\nu(x)$. Thus

$$\begin{aligned}&N_\nu(x)=[w_\nu'^2(x)+u_\nu'^2(x)]^{1/2}\qquad(-c_\nu\leqslant x\leqslant c_\nu)\\&N_\nu(x)=\left[\frac{u_\nu^2(x)w_\nu'^2(x)+w_\nu^2(x)u_\nu'^2(x)}{w_\nu(x)u_\nu(x)}\right]^{1/2}\qquad(c_\nu\leqslant x<+\infty).\end{aligned} \tag{2.32}$$

Evidently, $|w_\nu'(x)|\leqslant N_\nu(x)/E_\nu(x)$ for all $x\in[-c_\nu,+\infty)$. From the connection formulae (2.5) it follows $N_\nu(-x)=N_\nu(x)$ for $x\in[-c_\nu,c_\nu]$. In particular, from (2.6) and (2.32), we obtain

$$N_\nu(0)=\frac{2^{(\nu+1)/2}}{(2\pi)^{1/4}\Gamma^{1/2}(\nu+1)}\Gamma\left(1+\frac{\nu}{2}\right). \tag{2.33}$$

The product $M_\nu(0)N_\nu(0)$ of the values (2.16) and (2.33) is equal to unity exactly,

$$M_\nu(0)N_\nu(0)=1. \tag{2.34}$$

As to the explicit expressions for the function $\omega_\nu(x)$, they will not be used in the present paper, and so they are not given here.

The asymptotic form for $N_\nu(x)$, with $\nu\geqslant-1/2$ being fixed while $x\to+\infty$, is obtainable from the definition (2.32), on using the asymptotic representations (2.7) for the functions $w_\nu(x)$ and $u_\nu(x)$ along with the known relations [20, p 327] for their derivatives. As a result, we obtain

$$N_\nu(x)\sim\sqrt{\frac{x}{2}}\qquad(x\to+\infty). \tag{2.35}$$

The uniform asymptotic representation for $N_\nu(x)$, as $\nu\gg1$ while $x\in[0,+\infty)$, is readily obtained from the uniform asymptotic forms for the derivatives $w_\nu'(x)$ and $u_\nu'(x)$.

We have, for $\nu \gg 1$ and $x \in [0, +\infty)$,

$$w'_\nu(x) \sim \sqrt{\pi}\left[\frac{\frac{1}{4}x^2 - \nu - \frac{1}{2}}{\zeta(x)}\right]^{1/4} \mathrm{Ai}'(\zeta) \tag{2.36a}$$

$$u'_\nu(x) \sim \sqrt{\pi}\left[\frac{\frac{1}{4}x^2 - \nu - \frac{1}{2}}{\zeta(x)}\right]^{1/4} \mathrm{Bi}'(\zeta) \tag{2.36b}$$

where $\mathrm{Ai}'(\zeta)$ and $\mathrm{Bi}'(\zeta)$ are the derivatives of the Airy functions with respect to ζ. Substituting (2.36*a*) and (2.36*b*) in (2.32) yields

$$N_\nu(x) \sim \sqrt{\pi}\left[\frac{\frac{1}{4}x^2 - \nu - \frac{1}{2}}{\zeta(x)}\right]^{1/4} \mathrm{N}(\zeta) \tag{2.37}$$

with $\mathrm{N}(x)$ being the modulus function introduced in [10, p 396] relative to the derivatives of the Airy functions.

For every $\nu \geqslant -1/2$, we associate with the pair of functions $M_\nu(x)$ and $N_\nu(x)$ a positive parameter μ_ν defined by

$$\mu_\nu = \sup_{x\in[0,+\infty)} [N_\nu(x)M_\nu(x)]. \tag{2.38}$$

Taking into account the asymptotic relations (2.18) for $M_\nu(x)$ and (2.35) for $N_\nu(x)$, we find for every fixed $\nu \geqslant -1/2$

$$\lim_{x\to+\infty} [N_\nu(x)M_\nu(x)] = 1. \tag{2.39}$$

Therefore the right-hand side of (2.38) is bounded in magnitude for every finite $\nu \geqslant -1/2$. On the other hand, as $\nu \to +\infty$, the limiting value of μ_ν may be found by substituting uniform asymptotic representations (2.37) for $N_\nu(x)$ and (2.21) for $M_\nu(x)$, in the expression (2.38). We get

$$\lim_{\nu\to+\infty} \mu_\nu = \sup_{\zeta\in(-\infty,+\infty)} [\pi \mathrm{N}(\zeta)\mathrm{M}(\zeta)] = 1.060\,235 \tag{2.40}$$

correct to six decimal places.

The parameter μ_ν is a continuous function of ν. As ν ranges over the interval $[-1/2, +\infty)$, the corresponding values of μ_ν are confined to the segment $(1.036, 1.061)$. In particular, $\mu_\nu = 1.058\,049$ at $\nu = -1/2$, correct to six decimal places. The graph of μ_ν is plotted in figure 3 as a broken curve. The kink in the graph is due to the fact that the product $N_\nu(x)M_\nu(x)$ has two different local maxima on the positive real axis. The value of the product at one of those maxima monotonically decreases with increasing ν, while another maximum value of $N_\nu(x)M_\nu(x)$ monotonically increases with ν. At the point of the kink, the two local maximum values become equal.

2.4. Amplitude function associated with $w_\nu(x)$

In order to formulate sufficient conditions for correction terms (in asymptotic forms considered below) to be negligible, we shall have to compare those terms with the magnitude of the Weber function $w_\nu(x)$. We arrive at a suitable definition for the measure of the magnitude of $w_\nu(x)$ by introducing the *amplitude function* $\mathrm{Am}[w_\nu(x)]$ associated with $w_\nu(x)$. Let $x = x_\nu$ be the greatest positive zero of the function $u_\nu(x)$ (2.3)

$$\begin{aligned} &u_\nu(x) = 0 \qquad (x = x_\nu) \\ &u_\nu(x) > 0 \qquad (x > x_\nu). \end{aligned} \tag{2.41}$$

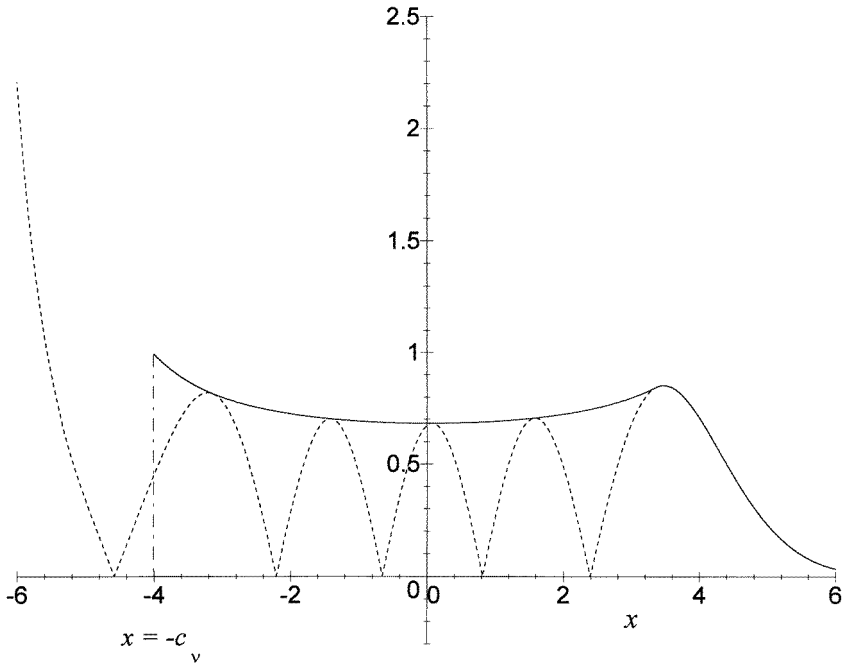

Figure 4. Graph of the amplitude function $\mathrm{Am}[w_\nu(x)]$ (full curve) for $\nu = 4.1$. The broken curve represents the absolute value $|w_\nu(x)|$ for the same ν.

From (2.10) and (2.15) we infer that $x_\nu < c_\nu$.

We define $\mathrm{Am}[w_\nu(x)]$ on the interval $x \in [-c_\nu, +\infty)$ as a continuous, positive function given by

$$\mathrm{Am}[w_\nu(x)] = \begin{cases} M_\nu(x) & \text{if } -c_\nu \leqslant x \leqslant x_\nu \\ w_\nu(x) & \text{if } x_\nu \leqslant x < +\infty. \end{cases} \tag{2.42}$$

Obviously, $|w_\nu(x)| \leqslant \mathrm{Am}[w_\nu(x)]$ for $x \in [-c_\nu, +\infty)$. For the rest of the real axis, i.e. for $x < -c_\nu$, an appropriate definition of the amplitude function is possible but not necessary for the purposes of the present paper. The graph of the amplitude function $\mathrm{Am}[w_\nu(x)]$ is plotted in figure 4 for $\nu = 4.1$, as a full curve. The broken curve in this figure represents the absolute value $|w_\nu(x)|$ for the same $\nu = 4.1$.

3. Bound-state problem and its asymptotic solution

3.1. Bound-state problem

Let us consider a particle with a mass m and total energy $E < 0$ which moves along the real x axis in a potential $U(x)$ that forms a well. We assume that (i) $U(x)$ is a real, continuous, and three times continuously differentiable function on the whole of the real axis; and that (ii) the function $U(x)$ tends to respective non-negative values U_- and U_+, as $x \to \pm\infty$, that is

$$\lim_{x\to-\infty} = U_- \geqslant 0 \qquad \lim_{x\to+\infty} = U_+ \geqslant 0. \tag{3.43}$$

Either, or both, of the values $U_{\pm}$ may be infinite. Let $U_{\min} < 0$ be the minimum value of the potential $U(x)$ on the real axis. Only the interval $U_{\min} < E < 0$ will be considered in what follows.

The wave function $\psi(x)$ that represents the particle's bound state in the potential well $U(x)$, satisfies the Schrödinger equation

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + p^2(x)\psi(x) = 0 \qquad \Big(\lim_{x\to\pm\infty}\psi(x) = 0\Big). \tag{3.44}$$

The function $p^2(x)$ in (3.44),

$$p^2(x) = 2m[E - U(x)] \qquad (\hbar = 1) \tag{3.45}$$

coincides with the square of the classical momentum of the particle for x satisfying $U(x) \leqslant E$. We restrict the ensuring analysis to energies $E \in (U_{\min}, 0)$ for which the equation $p^2(x) = 0$, considered on the real axis $-\infty < x < +\infty$, has two and only two simple, distinct, real roots $x = a$ and $x = b$

$$p^2(a) = p^2(b) = 0 \qquad (a < b) \tag{3.46}$$

such that $p^2(x) > 0$ if $a < x < b$, and $p^2(x) < 0$ if $x < a$ or $x > b$. We assume that $p(x) > 0$ for $a < x < b$. To simplify the reasoning, we may suppose that these conditions are fulfilled for *all* $E \in (U_{\min}, 0)$, though the final result (see theorem 2 in section 4) is not bound to the latter assumption.

3.2. Introduction of an asymptotic approach

In order to apply asymptotic methods in solving the Schrödinger equation, we have to specify a large parameter in the differential equation (3.44). An explicit specification of a large parameter in equation (3.44) is, however, not necessary at *this* stage of analysis. It will suffice if we assume the function $p^2(x)$ to be 'sufficiently smooth' on the real axis. The exact mathematical meaning of the latter property is defined below by (4.101). Specification of a large parameter for finite-range potentials is considered below in section 5.

Thus, we have to consider the problem of finding an asymptotic representation which should be valid uniformly with respect to all real x including the two turning points $x = a$ and $x = b$, for the wave function $\psi(x)$ that describes the particle's bound state in the potential $U(x)$. The appropriate functions to represent $\psi(x)$ in problems with two turning points, are the Weber parabolic cylinder functions [21–23].

3.2.1. Definition of the x–ξ mapping. Further analysis follows closely the reasoning of section 3 in [25]. We define a real, continuous, and strictly increasing function $\xi = \xi(x)$ that satisfies the equation

$$\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\right)^2 = \frac{p^2(x)}{\xi_0^2 - \xi^2} \tag{3.47}$$

on the real axis, with a real positive constant ξ_0. The constant ξ_0 is completely determined by equation (3.47) if we consider the latter along with the requirement that the derivative $\mathrm{d}\xi/\mathrm{d}x$ be finite, continuous, and positive on the real axis including at the two turning points $x = a$ and $x = b$, i.e.

$$\frac{\mathrm{d}\xi}{\mathrm{d}x} > 0 \qquad (-\infty < x < +\infty). \tag{3.48}$$

Thus we find

$$\xi_0^2 = \frac{2}{\pi}\int_a^b p(x)\,\mathrm{d}x. \tag{3.49}$$

The solution $\xi = \xi(x)$ of equation (3.47) is then found to be unique and determined by the following relations

(a) if $x \leqslant a$, then $\xi \leqslant -\xi_0$ and

$$\int_{\xi}^{-\xi_0} (\xi^2 - \xi_0^2)^{1/2}\,\mathrm{d}\xi = \int_x^a |p(x)|\,\mathrm{d}x \tag{3.50a}$$

(b) if $a \leqslant x \leqslant b$, then $-\xi_0 \leqslant \xi \leqslant \xi_0$ and

$$\int_{-\xi_0}^{\xi} (\xi_0^2 - \xi^2)^{1/2}\,\mathrm{d}\xi = \int_a^x p(x)\,\mathrm{d}x \tag{3.50b}$$

(c) if $x \geqslant b$, then $\xi \geqslant \xi_0$ and

$$\int_{\xi_0}^{\xi} (\xi^2 - \xi_0^2)^{1/2}\,\mathrm{d}\xi = \int_b^x |p(x)|\,\mathrm{d}x. \tag{3.50c}$$

As was proven by Langer [23], the function $\xi(x)$ defined by (3.50*a–c*) is continuous, strictly increasing, and thrice continuously differentiable on the whole of the real axis, if the above conditions upon the potential $U(x)$ are fulfilled. Thus the function $\xi(x)$ defines a one-to-one mapping of the x axis, $-\infty < x < +\infty$, onto the ξ axis, $-\infty < \xi < +\infty$.

While being strictly increasing, the function $\xi(x)$ has a unique zero $x = x_0$ on the real axis, such that $a < x_0 < b$. Let us take the point $x = x_0$ as the origin on the x axis, $x_0 = 0$. This choice is supposed to hold throughout the remaining part of the paper.

3.2.2. Specification of the parameter ν. For each E such that $U_{\min} < E < 0$, we define a real, continuous parameter $\nu = \nu(E)$

$$\nu + \tfrac{1}{2} = \frac{1}{\pi}\int_a^b p(x)\,\mathrm{d}x. \tag{3.51}$$

As E ranges over the interval $(U_{\min}, 0)$, the parameter $\nu(E)$ varies in the interval $(-1/2, \nu_{\max})$, where the (finite or infinite) limiting value $\nu_{\max}$ is given by

$$\nu_{\max} = -\frac{1}{2} + \frac{1}{\pi}\lim_{E\to 0-}\int_a^b p(x)\,\mathrm{d}x. \tag{3.52}$$

The parameter ν (3.51) is related to ξ_0 (3.49) by $\xi_0^2 = 2\nu + 1$.

3.2.3. Basic representation for recessive solutions. Next, let us consider the function

$$\phi_\nu(x) = \left[\frac{\xi_0^2 - \xi^2}{p^2(x)}\right]^{1/4} w_\nu\left(\xi\sqrt{2}\right) \tag{3.53}$$

where $w_\nu(x)$ is the Weber function defined by (2.2), $\xi = \xi(x)$ is given by the relations (3.50*a–c*), and ν is specified by (3.51). By direct differentiation we find that the function (3.53) satisfies the following differential equation

$$\frac{\mathrm{d}^2\phi_\nu}{\mathrm{d}x^2} + [p^2(x) + R(x)]\phi_\nu = 0 \tag{3.54}$$

where

$$R(x) = \frac{1}{2}\frac{|p(x)|''}{|p(x)|} - \frac{3}{4}\frac{|p(x)|'^2}{|p(x)|^2} + \frac{3\xi^2 + 2\xi_0^2}{4(\xi^2 - \xi_0^2)^2}\frac{p^2(x)}{\xi_0^2 - \xi^2} \tag{3.55}$$

$$= -(\xi')^{1/2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}(\xi')^{-1/2} \qquad \xi' \equiv \frac{\mathrm{d}\xi}{\mathrm{d}x} \tag{3.56}$$

and the prime denotes differentiating with respect to x.

Consider an *exact* solution $\psi_\nu^{(+)}(x)$ to the Schrödinger equation (3.44) that vanishes at positive infinity,

$$\lim_{x\to+\infty} \psi_\nu^{(+)}(x) = 0. \tag{3.57}$$

If $U(x)$, E and $\nu = \nu(E)$ are specified as indicated above, this solution exists for every $\nu > -1/2$ [24]. Let us try $\psi_\nu^{(+)}(x)$ as the sum

$$\psi_\nu^{(+)}(x) = \phi_\nu(x) + \delta_\nu^{(+)}(x) \tag{3.58}$$

where $\phi_\nu(x)$ is given by (3.53), with an additional term $\delta_\nu^{(+)}(x)$ satisfying

$$\lim_{x\to+\infty} \delta_\nu^{(+)}(x) = 0 \qquad \lim_{x\to+\infty} \frac{\mathrm{d}\delta_\nu^{(+)}(x)}{\mathrm{d}x} = 0. \tag{3.59}$$

We substitute the sum $\psi_\nu^{(+)}(x)$ (3.58) in the Schrödinger equation (3.44), this yields a differential equation for $\delta_\nu^{(+)}(x)$. Then we transform the latter to an equivalent integral equation for $\delta_\nu^{(+)}(x)$ while taking into account the boundary conditions (3.59). Finally, on putting $\delta_\nu^{(+)}(x)$ into the same form as $\phi_\nu(x)$ (3.53),

$$\delta_\nu^{(+)}(x) = \left[\frac{\xi_0^2 - \xi^2}{p^2(x)}\right]^{1/4} h_\nu^{(+)}(x) \tag{3.60}$$

we obtain an integral equation for the correction term $h_\nu^{(+)}(x)$

$$h_\nu^{(+)}(z) = \int_z^{+\infty} K_\nu(z, z_1)\left(\frac{R(z_1)}{|p(z_1)|}\frac{\mathrm{d}t}{\mathrm{d}z_1}\right)[w_\nu(z_1) + h_\nu^{(+)}(z_1)]\,\mathrm{d}z_1 \tag{3.61}$$

where we have denoted

$$z = z(x) \equiv \sqrt{2}\xi(x) \qquad z_1 = z_1(t) \equiv \sqrt{2}\xi(t). \tag{3.62}$$

In view of (3.51), the kernel $K_\nu(z, z_1)$ in (3.61) may be written as

$$K_\nu(z, z_1) = |\tfrac{1}{4}z_1^2 - \nu - \tfrac{1}{2}|^{1/2}[w_\nu(z)u_\nu(z_1) - u_\nu(z)w_\nu(z_1)] \tag{3.63}$$

where $w_\nu(z)$ and $u_\nu(z)$ are the Weber functions defined by (2.2) and (2.3). Let us investigate the integral equation (3.61).

3.2.4. Integral equation for the correction term $h_\nu^{(+)}(z)$. The proof for the existence and uniqueness of the solution $h_\nu^{(+)}(z)$ to equation (3.61), as well as the assessment of its magnitude, are based on the *theorem on singular integral equations* by Olver (see [10, theorem 10.1 in ch 6, p 217]). The purpose of the ensuing analysis is to show that the application of theorem 10.1 to the integral equation (3.61) results in the following.

Theorem 1. With the foregoing specifications in equation (3.61),

(i) for each $\nu > -1/2$, the integral equation (3.61) has a unique, continuous solution $h_\nu^{(+)}(z)$ on the interval $z \in [-c_\nu, +\infty)$ provided the integral

$$\mathrm{V}_+(z) = \int_z^{+\infty} \mathrm{d}z_1 \left|\frac{R(z_1)}{p(z_1)}\right| \frac{\mathrm{d}t}{\mathrm{d}z_1} \tag{3.64}$$

converges for all z in this interval;

(ii) the function $h_\nu^{(+)}(z)$, which satisfies (3.61), and its first derivative $\mathrm{d}h_\nu^{(+)}/\mathrm{d}z$, have the assessments

$$|h_\nu^{(+)}(z)| \leqslant g_\nu(z)[\mathrm{e}^{\sigma_\nu \mathrm{V}_+(z)} - 1]\,\mathrm{Am}[w_\nu(z)] \tag{3.65}$$

$$\left|\frac{\mathrm{d}h_\nu^{(+)}(z)}{\mathrm{d}z}\right| \leqslant \frac{N_\nu(z)}{E_\nu(z)}[\mathrm{e}^{\sigma_\nu \mathrm{V}_+(z)} - 1] \tag{3.66}$$

for $z \in [-c_\nu, +\infty)$.

In equations (3.65) and (3.66),

(iii) the functions $\mathrm{Am}[w_\nu(z)]$, $E_\nu(z)$ have been defined in section 2;

(iv) σ_ν is a finite, positive parameter defined by (2.23) ; its magnitude is of the order of unity for all $\nu > -1/2$ including in the limit $\nu \to +\infty$;

(v) $g_\nu(z)$ is a continuous positive function that is bounded in magnitude by a number of the order of unity for each $\nu > -1/2$, uniformly with respect to all $z \in [-c_\nu, +\infty)$. Moreover,

$$g_\nu(z) = 1 \qquad (-c_\nu \leqslant z \leqslant z_\nu) \qquad g_\nu(z) = \sqrt{2} \qquad (c_\nu \leqslant z < +\infty) \tag{3.67}$$

where z_ν is the greatest positive root of the equation $u_\nu(z) = 0$ with $u_\nu(z)$ defined by (2.3).

Proof. Let us apply theorem 10.1 [10, ch 6, p 217] to equation (3.61) considered on the interval $-c_\nu \leqslant z < +\infty$ of the real z axis. In the notation of theorem 10.1, we have $\alpha = +\infty$, $\beta = -c_\nu$, and

$$\begin{gathered}\phi(z_1) = \psi_0(z_1) = \frac{R(z_1)}{|p(z_1)|}\frac{\mathrm{d}t}{\mathrm{d}z_1} \qquad \psi_1(z_1) = 0 \qquad J(z_1) = w_\nu(z_1) \\ \Phi(z) = \Psi_0(z) = \mathrm{V}_+(z) \qquad \Psi_1(z) = 0.\end{gathered} \tag{3.68}$$

If the functions $w_\nu(z)$, $\phi(z)$, and $K_\nu(z, z_1)$ in equation (3.61) are specified as indicated above in this section, then the conditions (i)–(iv) of theorem 10.1 are fulfilled. Next, for $z \in [-c_\nu, +\infty)$, we can use the expressions (2.10) for the functions $w_\nu(x)$ and $u_\nu(x)$. On substituting them in (3.63), we obtain

$$\begin{aligned}|K_\nu(z, z_1)| = M_\nu(z)M_\nu(z_1)\left|\frac{z_1^2}{4} - \nu - \frac{1}{2}\right|^{1/2}\frac{E_\nu(z_1)}{E_\nu(z)} \\ \times \left|\cos\theta_\nu(z)\sin\theta_\nu(z_1) - \frac{E_\nu^2(z)}{E_\nu^2(z_1)}\sin\theta_\nu(z)\cos\theta_\nu(z_1)\right|.\end{aligned} \tag{3.69}$$

Taking into account that $z \leqslant z_1$ and hence $E_\nu(z) \leqslant E_\nu(z_1)$, we see that the factor on the second line of (3.69) is less than or equal to unity for all $z \in [-c_\nu, +\infty)$. Therefore, from equation (3.69) it follows

$$|K_\nu(z, z_1)| \leqslant P_\nu(z)Q_\nu(z_1) \qquad (-c_\nu \leqslant z \leqslant z_1 < +\infty) \tag{3.70}$$

where the functions $P_\nu(z)$ and $Q_\nu(z_1)$

$$P_\nu(z) = \frac{M_\nu(z)}{E_\nu(z)} \qquad Q_\nu(z_1) = M_\nu(z_1)E_\nu(z_1)\left|\frac{z_1^2}{4} - \nu - \frac{1}{2}\right|^{1/2} \tag{3.71}$$

satisfy the requirements of theorem 10.1. Using the expressions (3.71) for $P_\nu(z)$ and $Q_\nu(z_1)$, we see that the parameter κ_0 of theorem 10.1 coincides with σ_ν (2.23). Also, as long as

$$|w_\nu(z)| \leqslant \frac{M_\nu(z)}{E_\nu(z)} \qquad \text{for } -c_\nu \leqslant z < +\infty \tag{3.72}$$

using the expression (3.71) for $Q_\nu(z)$ yields an assessment for the second parameter κ of theorem 10.1, i.e. $\kappa \leqslant \sigma_\nu$. Hence, for every $\nu > -1/2$ *including* in the limit $\nu \to +\infty$, the condition (vi) of theorem 10.1 is fulfilled. The statement (i) of theorem 1 is thus proved. Furthermore, from theorem 10.2 [10, ch 6, p 218] we obtain the assessment for $h_\nu^{(+)}(z)$

$$|h_\nu^{(+)}(z)| \leqslant \frac{M_\nu(z)}{E_\nu(z)}[\mathrm{e}^{\sigma_\nu \mathrm{V}_+(z)} - 1] \qquad (-c_\nu \leqslant z < +\infty). \tag{3.73}$$

The latter relation is brought into its final form (3.65) by introducing the function $g_\nu(z)$ defined by

$$g_\nu(z) = \frac{M_\nu(z)}{E_\nu(z)\,\mathrm{Am}[w_\nu(z)]} = \begin{cases} 1 & \text{if } -c_\nu \leqslant z \leqslant z_\nu \\ \dfrac{M_\mu(z)}{w_\nu(z)} & \text{if } z_\nu \leqslant z \leqslant c_\nu \\ \sqrt{2} & \text{if } c_\nu \leqslant z < +\infty. \end{cases} \tag{3.74}$$

In a similar way, using the representations (2.31) for $w_\nu'(x)$ and $u_\nu'(x)$, we obtain the assessment (3.66) for the derivative $\mathrm{d}h_\nu^{(+)}(z)/\mathrm{d}z$. □

Taking into account (3.47) and (3.55), we bring the expression (3.64) into its final form

$$\mathrm{V}_+(x) = \int_x^{+\infty} \frac{\mathrm{d}x}{|\xi^2(x) - \xi_0^2|^{1/2}} \left| (\xi')^{-1/2} \frac{\mathrm{d}^2}{\mathrm{d}x^2}(\xi')^{-1/2} \right| \qquad (\xi' = \mathrm{d}\xi/\mathrm{d}x) \tag{3.75}$$

where $\xi_0^2 = 2\nu + 1$.

3.3. Recessive solutions and their matching

If $U(x)$, E, and $\nu = \nu(E)$ are specified as indicated in sections 3.1 and 3.2.2, then for *every* fixed $\nu > -1/2$, there exists an *exact* solution $\psi_\nu^{(+)}(x)$ of equation (3.44) which vanishes at *positive* infinity [24], and this solution is unique (apart from a constant factor). In view of (3.58), (3.53), and (3.60), it may be written as

$$\psi_\nu^{(+)}(x) = \left[\frac{\xi_0^2 - \xi^2}{p^2(x)}\right]^{1/4} [w_\nu(z) + h_\nu^{(+)}(z)] \qquad \Big(z = z(x) \equiv \sqrt{2}\xi(x)\Big). \tag{3.76}$$

From the assessments (3.65) and (3.66), we see that, for every $\nu > -1/2$, the magnitude of the correction term $h_\nu^{(+)}(z)$ in (3.76) is negligibly small on the interval $[-c_\nu, +\infty)$, as compared with the first term $w_\nu(z)$ in the square brackets of (3.76), $|h_\nu^{(+)}(z)| \ll \mathrm{Am}[w_\nu(z)]$, if the condition $\mathrm{V}_+(x) \ll 1$ is fulfilled for all x such that $z(x) \in [-c_\nu, +\infty)$ (i.e. for all $x \in [-\varsigma_\nu, +\infty)$, where $x = -\varsigma_\nu < 0$ is the (unique) root of the equation $z(x) = -c_\nu$). However, we cannot neglect $h_\nu^{(+)}(z)$ on the interval $(-\infty, -c_\nu)$ if ν assumes a non-negative integer value $\nu = n = 0, 1, \ldots$. Besides, for arbitrary ν, except for certain special values of the latter, the magnitude of $\psi_\nu^{(+)}(x)$ increases and is unbounded at *negative* infinity, as $x \to -\infty$.

On the other hand, with the same specifications in $U(x)$, E, and $\nu = \nu(E)$, for *every* fixed $\nu > -1/2$ there exists another *exact* solution $\psi_\nu^{(-)}(x)$ of the Schrödinger equation (3.44), the one which vanishes at *negative* infinity

$$\psi_\nu^{(-)}(x) = \left[\frac{\xi_0^2 - \xi^2}{p^2(x)}\right]^{1/4} [w_\nu(-z) + h_\nu^{(-)}(z)] \qquad (z = z(x) \equiv \sqrt{2}\xi(x)) \tag{3.77}$$

and this solution is also unique (within a constant factor). The correction term $h_\nu^{(-)}(z)$ in (3.77) vanishes at negative infinity along with its derivative, for every $\nu > -1/2$. In

just the same manner as considered above with regard to $h_\nu^{(+)}(z)$, we may prove that the correction term $h_\nu^{(-)}(z)$ in (3.77) is a continuous function on the interval $(-\infty, c_\nu]$ which is continuously differentiable on this interval and has the following assessments

$$|h_\nu^{(-)}(z)| \leqslant g_\nu(-z)[e^{\sigma_\nu V_-(x)} - 1]\,\mathrm{Am}[w_\nu(-z)] \qquad (-\infty < z \leqslant c_\nu) \tag{3.78a}$$

$$\left|\frac{dh_\nu^{(-)}(z)}{dz}\right| \leqslant \frac{N_\nu(-z)}{E_\nu(-z)}[e^{\sigma_\nu V_-(x)} - 1] \qquad (-\infty < z \leqslant c_\nu). \tag{3.78b}$$

In (3.78*a*, *b*), x is related to z by $z = z(x)$ whereas the function $V_-(x)$ is given by

$$V_-(x) = \int_{-\infty}^{x} \frac{dx}{|\xi^2(x) - \xi_0^2|^{1/2}} \left|(\xi')^{-1/2}\frac{d^2}{dx^2}(\xi')^{-1/2}\right| \qquad (\xi' = d\xi/dx). \tag{3.79}$$

From the latter assessments it follows that, for every fixed $\nu > -1/2$, the magnitude of the correction term $h_\nu^{(-)}(z)$ in (3.77) is negligibly small on the interval $(-\infty, c_\nu]$, as compared with the first term $w_\nu(-z)$ in the square brackets of (3.77) $|h_\nu^{(-)}(z)| \ll \mathrm{Am}[w_\nu(-z)]$, if $V_-(x) \ll 1$ for all x such that $z(x) \in (-\infty, c_\nu]$. However, we cannot neglect $h_\nu^{(-)}(z)$ on the interval $(c_\nu, +\infty)$ if ν takes on a non-negative integer value $\nu = n = 0, 1, \ldots$. Besides for arbitrary ν, except for certain special values of the latter, the magnitude of $\psi_\nu^{(-)}(x)$ increases and is unbounded at *positive* infinity, as $x \to +\infty$.

Let us now consider the pair of exact solutions (3.76) and (3.77). For *any* fixed $\nu > -1/2$, the first of them, $\psi_\nu^{(+)}(x)$, vanishes at positive infinity whereas the second one, $\psi_\nu^{(-)}(x)$, vanishes at negative infinity. If we find a specific value for ν such that the functions $\psi_\nu^{(+)}(x)$ and $\psi_\nu^{(-)}(x)$ become linearly dependent, then the two functions will represent *one and the same* solution to equation (3.44) (apart from constant factors), which vanishes both at positive and at negative infinities simultaneously. This specific solution is just the wavefunction $\psi(x)$ that represents the particle's bound state in the potential $U(x)$.

The necessary and sufficient condition for the functions $\psi_\nu^{(+)}(x)$ and $\psi_\nu^{(-)}(x)$ to be linearly dependent is that their Wronskian vanishes

$$W\{\psi_\nu^{(+)}(x), \psi_\nu^{(-)}(x)\} = \psi_\nu^{(+)}(x)\frac{d\psi_\nu^{(-)}(x)}{dx} - \psi_\nu^{(-)}(x)\frac{d\psi_\nu^{(+)}(x)}{dx} = 0. \tag{3.80}$$

Note that the Wronskian $W\{\psi_\nu^{(+)}(x), \psi_\nu^{(-)}(x)\}$ does not depend on x whatever $\nu > -1/2$ may be. Substituting the expressions (3.76) and (3.77) in (3.80), we obtain the equation for the energies of the bound states

$$W\{w_\nu(z), w_\nu(-z)\} + W\{w_\nu(z), h_\nu^{(-)}(z)\} + W\{h_\nu^{(+)}(z), w_\nu(-z)\} + W\{h_\nu^{(+)}(z), h_\nu^{(-)}(z)\} = 0. \tag{3.81}$$

In all terms of (3.81) the differentiation is performed with respect to z. According to the known expressions [20, p 327] for the Wronskians of the parabolic cylinder functions, and in view of the definition (2.2) of the function $w_\nu(x)$, we find that the first term on the left-hand side of (3.81) is equal to

$$W\{w_\nu(z), w_\nu(-z)\} = -\sin\pi\nu. \tag{3.82}$$

Taking into account that the expression on the left-hand side of (3.81), taken as a whole, does not depend on z, we see that the sum of the remaining terms on the left-hand side of (3.81) is a function only of ν, not of z. On designating the latter sum by $\Delta(\nu)$,

$$\Delta(\nu) = W\{w_\nu(z), h_\nu^{(-)}(z)\} + W\{h_\nu^{(+)}(z), w_\nu(-z)\} + W\{h_\nu^{(+)}(z), h_\nu^{(-)}(z)\} \tag{3.83}$$

we rewrite equation (3.81) in the form

$$\sin\pi\nu = \Delta(\nu) \tag{3.84}$$

where $\Delta(\nu)$ is a real, continuous function of $\nu > -1/2$. The system of two *exact* equations (3.51) and (3.84) determines the energies of the particle's bound states in the potential $U(x)$.

Obviously, an exact evaluation of the quantity $\Delta(\nu)$ amounts to solving the Schrödinger equation (3.44) exactly, which is not possible except for a few simplest potentials. However, it *is* possible to establish an upper bound to the magnitude of $\Delta(\nu)$, and thus to indicate sufficient conditions for $\Delta(\nu)$ to be negligible, with respect to a large variety of sufficiently smooth potentials $U(x)$.

3.4. Assessments for $\Delta(\nu)$

Consider the interval $[-c_\nu, c_\nu]$, with c_ν defined by equation (2.12), and let $z_a \in [-c_\nu, c_\nu]$ be an arbitrary point in this interval. We write the Wronskians on the right-hand side of (3.83) explicitly. Then we use the estimates (3.65), (3.66), (3.78*a*, *b*) for the correction terms $h_\nu^{(\pm)}(z)$ and their derivatives along with the assessments for $|w_\nu(z)|$ and $|w_\nu'(z)|$ that follow from (2.10) and (2.31), all of the estimates taken at the point z_a. As a result, from (3.83) we get the final assessment for $\Delta(\nu)$

$$|\Delta(\nu)| \leqslant 2\mu_\nu[\mathrm{e}^{2\sigma_\nu V_{\min}(\nu)} - 1]. \tag{3.85}$$

In (3.85), the parameters σ_ν and μ_ν have been defined by (2.23) and (2.38), respectively, whereas $V_{\min}(\nu)$ denotes the infinum

$$V_{\min}(\nu) = \inf_{z_a \in (-c_\nu, c_\nu)} \mathrm{V}_{\max}(z_a). \tag{3.86}$$

In the latter relation, $\mathrm{V}_{\max}(z_a)$ is the greater one of the two positive values $\mathrm{V}_+(x_a)$ (3.75) and $\mathrm{V}_-(x_a)$ (3.79), both taken at the point x_a such that $z_a = z(x_a)$,

$$\mathrm{V}_{\max}(z_a) = \max\{\mathrm{V}_-(x_a), \mathrm{V}_+(x_a)\}. \tag{3.87}$$

In view of the definitions (3.75) and (3.79), we have an obvious relation

$$V_{\min}(\nu) \leqslant \mathrm{V}_-(x_a) + \mathrm{V}_+(x_a) = \mathrm{E}(\nu) \tag{3.88}$$

where the function $\mathrm{E}(\nu)$

$$\mathrm{E}(\nu) = \int_{-\infty}^{+\infty} \frac{\mathrm{d}x}{|\xi^2(x) - \xi_0^2|^{1/2}} \left| (\xi')^{-1/2} \frac{\mathrm{d}^2}{\mathrm{d}x^2} (\xi')^{-1/2} \right| \qquad (\xi_0^2 = 2\nu + 1, \xi' = \mathrm{d}\xi/\mathrm{d}x) \tag{3.89}$$

is the error-control integral introduced in [25]; it is supposed to be convergent.

For the purpose of analytical investigation, the quantity $V_{\min}(\nu)$ in (3.85) may be replaced by its upper bound $\mathrm{E}(\nu)$ (3.89),

$$|\Delta(\nu)| \leqslant 2\mu_\nu[\mathrm{e}^{2\sigma_\nu \mathrm{E}(\nu)} - 1]. \tag{3.90}$$

However, if one is interested in *numerical* assessments, the use of equation (3.86) leads to somewhat better results. For instance, if the potential $U(x)$ is represented by an *even* function, $U(-x) = U(x)$, then taking $x_a = x_0 = 0$ yields $z_a = z(0) = 0$, whereupon the inequality (3.85) reduces to a simpler relation

$$|\Delta(\nu)| \leqslant 2[\mathrm{e}^{\sigma_\nu \mathrm{E}(\nu)} - 1] \tag{3.91}$$

without the factor 2 in the exponent, and with μ_ν replaced by unity in view of (2.34).

Let us introduce a positive parameter ρ_ν defined by

$$\rho_\nu = \begin{cases} 2[\mathrm{e}^{\sigma_\nu \mathrm{E}(\nu)} - 1] & \text{for even potentials } U(-x) = U(x) \\ 2\mu_\nu[\mathrm{e}^{2\sigma_\nu \mathrm{E}(\nu)} - 1] & \text{otherwise.} \end{cases} \tag{3.92}$$

Using the definition (3.92), we may write the assessments (3.90) and (3.91) as a single relation

$$|\Delta(\nu)| \leqslant \rho_\nu \qquad (\nu > -1/2). \tag{3.93}$$

Since σ_ν and μ_ν are continuous functions of $\nu \in [-1/2, +\infty)$ (see section 2), the parameter ρ_ν (3.92) is also continuous, except at singular points of the error-control integral $\mathrm{E}(\nu)$ (see [25, section 3]).

4. Equation for the energies of bound states

4.1. Solutions of the basic equation $\sin \pi\nu = \Delta(\nu)$

The equation (3.84) is to be solved for real $\nu > -1/2$. In turn, each real value $\nu > -1/2$ may be represented, in a unique fashion, as the sum

$$\nu = n + \delta \qquad (n = 0, 1, \ldots, -1/2 < \delta \leqslant 1/2) \tag{4.94}$$

of a non-negative integer $n \geqslant 0$ and a real number δ whose absolute value does not exceed one-half. On substituting (4.94) in (3.84), we bring equation (3.84) into an equivalent form

$$\delta = \frac{(-1)^n}{\pi} \arcsin \Delta(n + \delta) \qquad (n = 0, 1, \ldots, -1/2 < \delta \leqslant 1/2). \tag{4.95}$$

This formula defines a sequence of mutually independent equations numbered by n; each one of them is to be solved for real $\delta \in (-1/2, 1/2]$. Let $\delta = \delta_n$ be a solution (if it exists) of equation (4.95) for given n. Our purpose is now to extract all possible information on the solutions of equation (4.95) which is available in view of the established properties of the function $\Delta(n + \delta)$. First, the *existence* of solutions to equation (4.95) is to be investigated.

4.1.1. Existence and uniqueness of solutions. Let us fix a non-negative integer $n \geqslant 0$, and let $\varepsilon > 0$ be a positive number such that $\varepsilon < 1/2$. With the given integer n we associate a non-negative parameter $\varrho_n(\varepsilon)$ by

$$\varrho_n(\varepsilon) = \sup_{\delta \in (-\varepsilon, \varepsilon)} \rho_{n+\delta} \qquad (n \geqslant 0) \tag{4.96}$$

where ρ_ν was defined by (3.92) (we distinguish between the letters ρ and ϱ).

The sufficient condition for equation (4.95) to have a real root $\delta = \delta_n$ in the interval $(-\varepsilon, \varepsilon)$, is

$$\varrho_n(\varepsilon) < \sin \pi\varepsilon. \tag{4.97}$$

Indeed, from (4.95), (3.93), (4.97), and (4.96) we find

$$\frac{1}{\pi} \arcsin |\Delta(n + \delta)| \leqslant \frac{1}{\pi} \arcsin \rho_{n+\delta} \leqslant \frac{1}{\pi} \arcsin \varrho_n(\varepsilon) < \varepsilon \qquad (-\varepsilon \leqslant \delta \leqslant \varepsilon). \tag{4.98}$$

Hence, as the first member δ of equation(4.95) ranges over the closed interval $[-\varepsilon, \varepsilon]$, the second member of this equation varies continuously in such a manner that all its values remain within the same interval $(-\varepsilon, \varepsilon)$. Consequently, if the condition (4.97) is satisfied for the given integer $n \geqslant 0$, then, for this n, equation (4.95) has at least one real solution $\delta = \delta_n$ such the $|\delta_n| < \varepsilon$. In particular, taking in (4.97) and (4.96) $\varepsilon \ll 1$, we see that the sufficient condition for equation (4.95) to have a solution $\delta = \delta_n$ such that $|\delta_n| \ll 1$, is $\rho_n \ll 1$ or, in view of the definition (3.92), $\mathrm{E}(n) \ll 1$, provided the error-control integral $\mathrm{E}(\nu)$ (3.89) is a continuous function at $\nu = n$.

The *uniqueness* of the solution δ_n cannot be established on the basis of the single relation (3.93). In addition to the latter, a proper assessment for the derivative $\mathrm{d}\Delta(\nu)/\mathrm{d}\nu$ would also be needed. The derivation of such assessment should be a subject of special discussion. From a mathematical standpoint, there is no general reason to rule out the possibility of more than one solution to equation (4.95) with one and the same integer $n \geqslant 0$, for some sophisticated potentials. However, even if, for some $n \geqslant 0$, equation (4.95) has several different roots $\delta = \delta_n^{(j)}$, $j = 1, 2, \ldots, j_n$, all of them have none the less the same assessment (4.100) (see below) and hence are small under the same condition (4.101). In what follows, we restrict ourselves to the case of a single solution $\delta = \delta_n$ for each non-negative integer $n \geqslant 0$. This is the most probable situation that is found in known applications of the Bohr–Sommerfeld formula to reasonable physical problems.

4.1.2. Remarks on numerical assessment of solutions. In the previous section, we have addressed the problem of establishing sufficient conditions (upon $U(x)$) for the root $\delta = \delta_n$ of equation (4.95) to fall into the prescribed interval. There is an inverse problem, namely, that of determining the bounds for the values of the root δ_n, *if it exists*, for a *specific* potential $U(x)$ and for given integer $n \geqslant 0$.

To get *numerical* assessments, we have to specify the choice of ε in (4.96) for each possible integer $n \geqslant 0$ while taking into account singularities of the error-control integral. In the absence of any further restrictions on the potential $U(x)$, the parameter ε may be specified as follows. Let $n_{\max}$ be the (finite or infinite) integer part of the number $\nu_{\max}$ defined by (3.52). If $\nu_{\max}$ is finite, then $\delta_{\max}$ denotes its (non-negative) fractional part. If $n_{\max} \geqslant 1$, then for $n = n_{\max}$ we set $\varepsilon_n = \delta_{\max}/2$. If $n_{\max} > 1$, then with each positive integer $n = 1, 2, \ldots, n_{\max} - 1$, we associate $\varepsilon_n = 1/2$. Finally, to define the parameter ε_0 for $n = 0$, we take into account the fact that the uncertainty principle imposes a finite lower bound to possible values of the ground-state energy E_0, namely, $E_0 - U_{\min} \geqslant \eta > 0$. The lower bound η may be estimated by standard methods of quantum mechanics (see, for example, problem 2 for the harmonic oscillator in [27, section 23]). Substituting the estimated lowest possible value of $E_0 = E_0(\eta)$ in (3.51) with $\nu = \delta$, we obtain the lower bound $\delta = \delta_\eta > -1/2$ for possible values of δ. Then we set $\varepsilon_0 = \delta_\eta$, for $n = 0$. As a result, the parameter ε in (4.96) is defined for each $n = 0, 1, \ldots, n_{\max}$. Let us denote $\varrho_n = \varrho_n(\varepsilon_n)$. Using inequality (3.93) along with (3.92), from equation (4.95) we obtain the assessment (4.100) (see below) for the root $\delta = \delta_n$ of equation (4.95) (if it exists in the related interval $(-\varepsilon_n, \varepsilon_n)$), the assessment being valid for each $n = 0, 1, \ldots, n_{\max}$, such that $\varrho_n < 1$. Note that, for $n = 1, 2, \ldots, n_{\max} - 1$ (if $n_{\max} > 1$), the condition $\varrho_n < 1$ is sufficient for equation (4.95) to have at least one real root $\delta = \delta_n$ such that $|\delta_n| < \frac{1}{2}$.

In general, if a particle's energy E is not too close to the singular points of the error-control integral $\mathrm{E}(\nu)$ (most often the endpoints of the interval $(U_{\min}, 0)$), then the parameter ρ_ν (3.92) is a smooth function of ν. Therefore, finding the maximum value of $\rho_{n+\delta}$ in (4.96) over the corresponding interval ($|\delta| \leqslant \varepsilon_n$), for a given integer $n \geqslant 0$, generally presents no great problem. Even neglecting δ in $\rho_{n+\delta}$ completely (which amounts to replacing ϱ_n in (4.100) by ρ_n from (3.92) with $\nu = n$), would often result in no appreciable change in the numerical value of ϱ_n. For this reason, the formulae (4.100) and (3.92) provide a convenient way of assessing the correction term δ_n in the exact equation (4.99) even if the error-control integral (3.89) is (less than or) of the order of unity.

4.2. Exact equation for the energies of bound states

Substituting the real root $\delta = \delta_n$ of equation (4.95), for each $n \geqslant 0$, in the relation (4.94) for ν, and taking into account the definition of ν (3.51), we obtain an *exact* equation for the energies of the bound states

$$\frac{1}{\pi}\int_a^b p(x)\,\mathrm{d}x = n + \tfrac{1}{2} + \delta_n \qquad (n = 0, 1, \ldots, n_{\max}). \tag{4.99}$$

As was shown in section 4.1.2, the term δ_n in equation (4.99) has the assessment

$$|\delta_n| \leqslant \frac{1}{\pi}\arcsin \varrho_n \qquad (n = 0, 1, 2, \ldots, n_{\max}) \tag{4.100}$$

provided $\varrho_n < 1$, where $\varrho_n = \varrho_n(\varepsilon_n)$ was defined by (4.96) with $\varepsilon = \varepsilon_n$ as specified in section 4.1.2 (if $\varrho_n \geqslant 1$, then we cannot expect the Bohr–Sommerfeld formula to be a good approximation). In view of the results obtained above and, in particular, in section 4.1.1, we have the following.

Theorem 2. Under the above hypotheses upon the potential $U(x)$, for a given integer $n, n = 0, 1, 2, \ldots, n_{\max}$, the solution of the bound-state problem (3.44) exists, while the energy $E = E_n$ of the nth bound state satisfies equation (4.99) with $|\delta_n| \ll 1$, if the error-control integral $\mathrm{E}(\nu)$ (3.89), taken at $\nu = n$, is small compared with unity

$$\mathrm{E}(n) \ll 1 \tag{4.101}$$

provided the function $\mathrm{E}(\nu)$ is continuous at $\nu = n$. Moreover, the term δ_n in (4.99) has the assessment

$$|\delta_n| \leqslant A_n \mathrm{E}(n) + O(\mathrm{E}^2(n)). \tag{4.102}$$

The coefficient $A_n = 4\sigma_n\mu_n/\pi$, with σ_n and μ_n defined by (2.23) and (2.38), respectively, does not depend on $U(x)$ and is of the order of unity for *all* $n \geqslant 0$. In particular, $A_0 = 1.382\,405$ for $n = 0$, whereas A_n attains its maximum $A_\infty = 1.403\,287$ in the limit $n \to \infty$, correct to six decimal places. For even functions $U(-x) = U(x)$, the assessment (4.102) may be sharpened on replacing A_n by $B_n = 2\sigma_n/\pi$.

The expression for A_n in (4.102) was obtained from the first-order term in the expansion of ρ_ν (3.92) in powers of $\mathrm{E}(\nu)$.

Hence, under the condition (4.101) the equation (4.99) reduces to the conventional Bohr–Sommerfeld quantization formula. Furthermore, the relation (4.101) establishes the sufficient condition for the Bohr–Sommerfeld formula to be extended to lower integers $n \sim 1$, including the smallest one $n = 0$ if $\mathrm{E}(0) \ll 1$.

In view of theorem 1 (see section 3.2.4), the condition (4.101) is also sufficient for the correction terms $h_\nu^{(\pm)}(z)$ in the exact wavefunctions (3.76) and (3.77) to be neglected in comparison with the corresponding terms $w_\nu(\pm z)$, $|h_\nu^{(\pm)}(z)| \ll \mathrm{Am}[w_\nu(\pm z)]$, uniformly for z in the respective overlapping intervals $[-c_\nu, +\infty)$ and $(-\infty, c_\nu]$. At the same time, rejecting the term δ_n in equation (4.99) (if (4.101) is fulfilled) turns the resulting Bohr–Sommerfeld formula into the condition for the functions $w_\nu(\pm z)$ to be linearly dependent. As a result, the uniform asymptotic representation for the particle's bound state $\psi_n(x)$ related to the nth energy level E_n, is given on the whole of the real axis by

$$\psi_n(x) \sim \left[\frac{2n + 1 - \xi^2}{p^2(x)}\right]^{1/4} w_n\left(\xi\sqrt{2}\right) \qquad (\mathrm{E}(n) \ll 1, -\infty < x < \infty) \tag{4.103}$$

where $w_\nu(x)$ is the Weber function defined by (2.2) whereas the function $\xi = \xi(x)$ is determined by (3.50*a–c*) with $\xi_0^2 = 2n + 1$.

As an example, for harmonic oscillator $U(x) = m\omega^2 x^2/2$, and from (3.50*a–c*) we find $\xi(x) = x\sqrt{m\omega/\hbar}$ (cf [27] equation (23.7)), so the error-control integral (3.89) *vanishes* identically and in (4.99) $\delta_n = 0$ for all $n \geqslant 0$. Hence, for the harmonic oscillator the Bohr–Sommerfeld formula turns out to be exact for all $n \geqslant 0$, in accordance with the well known fact. Moreover, on writing $\hbar$ explicitly, for $E = E_n = \hbar\omega(n + 1/2)$ we have $p^2(x) = [2n + 1 - x^2 m\omega/\hbar](m\omega/\hbar)$ so (4.103) yields the exact wavefunction for the nth bound state on the whole of the real axis

$$\psi_n(x) = \left(\frac{\pi\hbar}{4m\omega}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} \exp\left(-x^2\frac{m\omega}{2\hbar}\right) H_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right) \tag{4.104}$$

which coincides with the known expression (23.12) in [27] multiplied with $(\pi\hbar/2m\omega)^{1/2}$.

5. Finite-range potentials

5.1. Scaling property of the error-control integral

Let us consider an important particular case when there is just a single, finite length scale l associated with the potential $U(x)$. This means that, in addition to its properties assumed above in section 3.1, the function $U(x)$ vanishes as $x \to \pm\infty$, and it is integrable over the real axis. The latter property allows us to define the length scale l by

$$l = \frac{1}{|U_0|}\left|\int_{-\infty}^{+\infty} U(x)\,\mathrm{d}x\right| \tag{5.105}$$

where U_0 is the typical value of the function $U(x)$ on the real axis. We assume that there are no other length scales associated with $U(x)$. Hence the function $U(x)$ may be written as

$$U(x) = U_0 f\left(\frac{x}{l}\right) \qquad (U_0 < 0) \tag{5.106}$$

where $f(x)$ is a generic designation for a function of just one variable. We denote by k_0 the typical wave number associated with the potential $U(x)$, that is,

$$k_0 = \sqrt{2m|U_0|} \qquad (\hbar = 1). \tag{5.107}$$

Let $k = \sqrt{2m|E|}$ be the wave number of the particle with the total energy E.

There is an important property the error-control integral has with respect to finite-range potentials. Indeed, equations (3.49), (3.50*a–c*) show that $\xi = \xi(x)$ is a homogeneous function of the order 1/2 with respect to scaling transformations of a particle's momentum $p(x)$†. This means that multiplying $p(x)$ with a constant factor $\alpha > 0$ entails multiplying $\xi(x)$ by $\alpha^{1/2}$. Since $p(x)$ contains the parameter $k_0 l$ only as a factor, the function $\xi(x)$ is proportional to $\sqrt{k_0 l}$. The formula (3.89) then shows the error-control integral to be a function of the form

$$\mathrm{E}(\nu) = \frac{1}{k_0 l} f\left(\frac{k}{k_0}\right) \equiv \frac{\hbar}{l\sqrt{2m|U_0|}} f\left(\frac{k}{k_0}\right). \tag{5.108}$$

Note that the large parameter designated by u in reference [19] may be identified with $k_0 l$ in problems with finite-range potentials in quantum mechanics (cf [26]). For finite-range potentials, from theorem 2 in section 4.2 we obtain the following.

† In fact, this is true with respect to more general scaling transformations of a particle's *classical action*. Indeed, equations (3.50*a–c*) define $\xi(x)$, for all x, as a function of just two variables $\int_a^b p(x)\mathrm{d}x$ and $\int_a^x |p(x)|\,\mathrm{d}x$ so there is no *direct* dependence of $\xi(x)$ on x.

Theorem 3. For finite-range potentials $U(x)$ as defined above, the sufficient condition for the error term δ_n in equation (4.99) to be negligible ($|\delta_n| \ll 1$) uniformly for $n \in [0, n_m]$ with a positive integer $n_m < n_{\max}$ is $k_0 l \gg 1$ or, written explicitly, $\overline{h} \ll l\sqrt{2m|U_0|}$, provided the error-control integral $\mathrm{E}(\nu)$ (3.89) is a continuous function in the closed interval $0 \leqslant \nu \leqslant n_m$.

5.2. Comparison with a known exact solution

Consider, as an example, the problem of determining the energies E_n of a particle's bound states in a (finite-range) potential well

$$U(x) = \frac{U_0}{\cosh^2(x/l)} \qquad (U_0 < 0). \tag{5.109}$$

For the potential (5.109), the error-control integral (3.89) has been calculated numerically as a function of the parameter kl, for $k_0 l = 10$, by performing direct numerical integration in (3.89). The graph of the function $\mathrm{E}(kl)$ was plotted as a broken curve in figure 2 of [25]. The graph shows a strong singularity of the function $\mathrm{E}(kl)$ in the range of low energies,

$$\mathrm{E}(kl) \sim \frac{1}{3kl} \qquad (kl \to 0+) \tag{5.110}$$

as well as a much weaker logarithmic singularity of this function near the bottom of the potential well,

$$\mathrm{E}(kl) \sim \frac{1}{4k_0 l}|\ln(k_0 l - kl)| \qquad (kl \to k_0 l - 0). \tag{5.111}$$

At the same time, in a wide range inside the interval $(0, k_0 l)$, the values of $\mathrm{E}(kl)$ are of the order of $1/(k_0 l)$. For instance, in figure 2 of [25], the function $\mathrm{E}(kl)$ attains its minimum value $\mathrm{E}_{\min} = 0.1376$ at $kl = 6.0898$, correct to four decimal places. All those features of the function $\mathrm{E}(kl)$ are found to be in complete agreement with the general properties of the error-control integral, which have been established in [25, section 3]. In view of equations (5.110) and (5.111), the condition $\mathrm{E}(\nu) \ll 1$ for the Bohr–Sommerfeld formula to be valid, will be fulfilled for all $E \in (-|U_0|, 0)$ if, first, the parameter $k_0 l$ is large compared with unity $k_0 l \gg 1$, and secondly, the particle's energy E is not too close to the endpoints of the interval $(-|U_0|, 0)$ i.e. $|\ln(k_0 l - kl)| \ll k_0 l$ and $kl \gg 1$.

On calculating the phase integral in equation (4.99) explicitly, we obtain the exact equation for the energies of the bound states in the potential (5.109)

$$\frac{1}{\pi}\int_a^b p(x)\,\mathrm{d}x = k_0 l - kl = n + \tfrac{1}{2} + \delta_n \qquad (n = 0, 1, \ldots). \tag{5.112}$$

It is easily seen that the condition $k_0 l \gg 1$ is sufficient for the correction term δ_n on the right-hand side of (5.112) to be negligible for *all* lower integers $n = 0, 1, \ldots$. Indeed, assume $k_0 l \gg 1$ and suppose that $|\delta_n| \ll 1$ in (5.112). Then, for all those integers, the difference $k_0 l - kl$ in (5.112) is bounded from zero by a number that is nearly equal to 1/2. In view of equation (5.111), the condition (4.101), which makes neglecting the term δ_n legitimate, will be satisfied for all lower integers $n \geqslant 0$ as long as $k_0 l \gg 1$. The hypothesis $|\delta_n| \ll 1$ is thus verified. In particular, for $n = 0$, substituting the calculated numerical values of $\mathrm{E}(0)$ in the relation (4.102) yields the assessments for δ_0

$$|\delta_0| \leqslant \frac{1.1783}{k_0 l} \qquad (k_0 l = 10, \mathrm{E}(0) = 0.1772,\ \frac{1}{\pi}\arcsin\rho_0 = 0.1333) \tag{5.113a}$$

$$|\delta_0| \leqslant \frac{1.5655}{k_0 l} \qquad (k_0 l = 100, \mathrm{E}(0) = 0.0235,\ \frac{1}{\pi}\arcsin\rho_0 = 0.0159) \tag{5.113b}$$

correct to four decimal places. In fact, the actual numbers in the numerators of the latter relations, as obtained from the exact solution of the problem [27], are found to be even less, i.e. 0.1249 and 0.1250, respectively.

Hence, if the potential (5.109) satisfies $k_0 l \gg 1$, then the Bohr–Sommerfeld quantization formula for this potential is applicable to the range of lower quantum numbers, to begin at the smallest one $n = 0$. On neglecting the term δ_n on the right-hand side of (5.112), we obtain approximate values $E_n^{\sim}$ for the energies of the bound states

$$E_n^{\sim} = -\frac{\hbar^2}{2ml^2}[k_0 l - (n + \tfrac{1}{2})]^2 \qquad (n = 0, 1, \ldots). \tag{5.114}$$

The meaning of the condition $k_0 l \gg 1$ becomes quite clear if we compare the approximate values $E_n^{\sim}$ given by equation (5.114) with the exact ones [27]

$$E_n = -\frac{\hbar^2}{2ml^2}\left[\sqrt{(k_0 l)^2 + \tfrac{1}{4}} - (n + \tfrac{1}{2})\right]^2 \qquad (n = 0, 1, \ldots). \tag{5.115}$$

It is readily seen that, for each $n \geqslant 0$, the approximate value $E_n^{\sim}$ (5.114) is formally obtained from the corresponding exact value E_n (5.115) by neglecting the number 1/4 under the sign of the square root in the brackets on the right-hand side of (5.115). Neglecting the term 1/4 in comparison with $k_0 l$ is, indeed, legitimate as long as the condition $k_0 l \gg 1$ is fulfilled, except, possibly, for very large numbers n, when the difference between the two large terms in the square brackets of (5.115) may become small compared with each one of the terms.

The exact expression for correction term δ_n in (5.112)

$$\delta_n = k_0 l + \sqrt{(k_0 l)^2 + \tfrac{1}{4}} \qquad (n = 0, 1, \ldots) \tag{5.116}$$

is found to be independent of the quantum number n, and $\delta_n \in (-1/2, 0)$ for all $k_0 l > 0$. In particular, for large $k_0 l \gg 1$, δ_n is inversely proportional to $k_0 l$

$$\delta_n \sim -\frac{1}{8}\frac{1}{k_0 l} \qquad (k_0 l \gg 1) \tag{5.117}$$

which is in accordance with the relation (4.102) and the scaling property (5.108) of the error-control integral.

In the range of large quantum numbers $n \gg 1$, where $kl \ll 1$, the estimated upper bound to the magnitude of the correction term δ_n in equation (5.112), as found from the assessment (4.100), turns out to be much greater than the actual values given by (5.116), or (5.117). To get insight into the meaning of this fact, let us note that the singularity of the type $1/(kl)$, as given by equation (5.110), comes from the integration in (3.89) over the range of large x, $|x| \gg l$, i.e. *only* from the exponential tails of the potential $U(x)$ (5.109). For this reason, the use of the relation (4.100) along with the expression (5.110) for the error-control integral yields an assessment for δ_n that refers, in fact, to a *set* of potentials that vanish exponentially as $|x| \to \infty$ while being quite different at finite $|x| \leqslant l$. On the other hand, the error term δ_n in equation (5.112) is sensitive to the detailed behaviour of the function $U(x)$ in the region $|x| \leqslant l$. It is, therefore, quite possible that the actual value of δ_n relative to a particular representative of the set of exponentially vanishing potentials, happens to be much smaller than its estimate given by a general assessment with respect to the set as a whole. That the singular behaviour (5.110) of the error-control integral, in the range of small kl, is not a spurious one, and happens not by chance, may be seen from the analysis of the related tunnelling problem for the potential (5.109) with $U_0 > 0$. In the latter problem, the restriction $kl \gg 1$, which is imposed by (5.110) along with the condition $\mathrm{E}(kl) \ll 1$ (4.101), was found to be quite essential for the semiclassical approach to be

valid [25]. In other words, the particular concourse of circumstances that caused the term δ_n to be exceptionally small in the bound-state problem for the potential (5.109), does not occur in the related tunnelling problem for the same potential.

It should be noted, in this respect, that the rigorous mathematical theorems [8–10] on the asymptotic validity of the Bohr–Sommerfeld formula, which establish the proof for the fact that the correction term δ_n in (4.99) vanishes in the limit of large quantum numbers n,

$$\delta_n = O\left(\frac{1}{k_n}\right) \qquad \text{as } n \to +\infty \qquad \left(k_n = \sqrt{2m|E_n|}\right) \tag{5.118}$$

are *essentially* based on the assumption that the potential $U(x)$ tends to positive *infinity* as $|x| \to \infty$. Those theorems do not apply to smooth potentials that *vanish* at infinity while having long-range tails. For such potentials, the semiclassical approximation may not be valid in the range of extremely low energies [27, section 46]. Indeed, it is readily seen that, for the potential (5.109), the integral $\int F^2/(8p^5)\,\mathrm{d}x$ that appears as the third term of the WKB expansion in the square brackets of equation (46.11) in [27] has a singularity of the type $1/(kl)$ as $kl \to 0$, i.e. just the same as the one given by (5.110). For this reason, the corresponding WKB correction term cannot be neglected for $kl \ll 1$. This means that quantum effects are essential for slow-moving particles in smooth potentials that vanish at infinity.

6. Connection to the WKB approximation

Let us consider the positive real axis $0 \leqslant x < +\infty$, with the origin $x = 0$ chosen as specified in section 3.2.1. There is only one turning point $x = b$ in the interval $[0, +\infty)$. If the condition $\mathrm{E}(n) \ll 1$ (4.101) is fulfilled for some fixed integer $n \geqslant 0$, then the correction term $h_n^{(+)}(x)$ on the right-hand side of (3.76) is negligible *uniformly* with respect to all real $x \in [0, +\infty)$. Therefore the particle's bound state $\psi_n(x)$ related to the given number n may be asymptotically represented, for $x \in [0, +\infty)$, by

$$\psi_n(x) \sim \left[\frac{\xi_0^2 - \xi^2}{2p^2(x)}\right]^{1/4} w_n\left(\xi\sqrt{2}\right) \qquad (\mathrm{E}(n) \ll 1, \xi_0^2 = 2n+1) \tag{6.119}$$

where $\xi = \xi(x)$ is defined by (3.50*a–c*). If n is also large $n \gg 1$, then the use of the uniform asymptotic form (2.8) along with (2.9) yields

$$w_n\left(\xi\sqrt{2}\right) \sim \sqrt{\pi}\left[\frac{2\zeta}{\xi^2 - \xi_0^2}\right]^{1/4} \mathrm{Ai}(\zeta) \qquad (n \gg 1, x \geqslant 0) \tag{6.120}$$

where the function $\zeta = \zeta(x)$ is given by

$$\tfrac{2}{3}[\zeta(x)]^{3/2} = \int_{\xi_0}^{\xi(x)} (\xi^2 - \xi_0^2)^{1/2}\,\mathrm{d}\xi = \int_b^x |p(x)|\,\mathrm{d}x \qquad (x \geqslant b) \tag{6.121a}$$

$$\tfrac{2}{3}[-\zeta(x)]^{3/2} = \int_{\xi(x)}^{\xi_0} (\xi_0^2 - \xi^2)^{1/2}\,\mathrm{d}\xi = \int_x^b p(x)\,\mathrm{d}x \qquad (0 \leqslant x \leqslant b). \tag{6.121b}$$

On substituting (6.120) in (6.119), we get

$$\psi_n(x) \sim \sqrt{\pi}\left[\frac{-\zeta(x)}{p^2(x)}\right]^{1/4} \mathrm{Ai}(\zeta) \qquad (\mathrm{E}(n) \ll 1, n \gg 1, x \geqslant 0). \tag{6.122}$$

If, in addition to $n \gg 1$, the integrals on the right-hand sides of (6.121) are also large, then the Airy function in (6.122) may be replaced by its own asymptotic form. As a result, the

formula (6.119) for the wave function $\psi_n(x)$ reduces to simple WKB expressions

$$\psi_n(x) \sim \frac{1}{\sqrt{p(x)}} \cos\left(\int_x^b p(x)\,\mathrm{d}x - \frac{\pi}{4}\right) + O\left(\frac{1}{n}\right)$$
$$\left(n \gg 1, 0 \leqslant x < b, \int_x^b p(x)\,\mathrm{d}x \gg 1\right)$$
$$\psi_n(x) \sim \frac{1}{2\sqrt{|p(x)|}} \exp\left(-\int_b^x |p(x)|\,\mathrm{d}x\right) + O\left(\frac{1}{n}\right)$$
$$\left(n \gg 1, x > b, \int_b^x |p(x)|\,\mathrm{d}x \gg 1\right)$$

in complete agreement with the known WKB connection formulae [27, section 47].

In section 2.2, it was shown that, as $\nu \to +\infty$, the parameter σ_ν (2.23) tends to the number λ introduced in reference [10, p 397] relative to the Airy functions. Moreover, it may be shown that, for large $\nu \gg 1$, the function $\mathrm{V}_+(x)$, which was defined above by (3.75), reduces to the variational operator $V_{x,\infty}(H)$ introduced in [10, ch 11, section 3] relative to the Airy functions, with $H = H(x)$ being the *error-control function* given by equation (3.08) (with $g = 0$) in ch 11 of the same reference. Namely, we find

$$\mathrm{V}_+(x) = V_{x,\infty}(H) + O\left(\frac{1}{\nu}\right) \qquad (\nu \gg 1, 0 \leqslant x < +\infty). \tag{6.123}$$

As a result, for large $\nu \gg 1$ and $x \in [0, +\infty)$, the assessments (3.65) and (3.66) obtained above in section 3.2.4 go over into the estimates (3.11) of the basic theorem (3.1) in [10, ch 11, section 3] which determines the validity of uniform asymptotic representations in terms of the Airy functions in problems with a *single* turning point and, in particular, the error bounds for the formula (6.122).

7. Discussion and conclusions

The above analysis shows that the exact equation (4.99) for the energies E_n of bound states reduces to the Bohr–Sommerfeld quantization formula if the condition $\mathrm{E}(n) \ll 1$ (4.101) is fulfilled. This condition is essentially different from the conventional WKB requirement $n \gg 1$, i.e. from the requirement that the Sommerfeld phase integral be large $\int_a^b p(x)\,\mathrm{d}x \gg 1$. Namely, the error-control integral may be small $\mathrm{E}(\nu) \ll 1$ *even* if the parameter ν is of the order of unity or less. This means that the Bohr–Sommerfeld formula holds true with the accuracy of the *post-classical approximation* [25], not merely with the accuracy of the WKB approximation.

Potentials for which the Bohr–Sommerfeld quantization formula is extendible to lower quantum numbers, are not at all exceptional ones. The sufficient condition $\mathrm{E}(n) \ll 1$ (4.101) for the Bohr–Sommerfeld formula to be extended to lower quantum numbers $n \sim 1$, may easily be satisfied for sufficiently smooth potentials $U(x)$ provided the second derivative $U''(x_m)$, taken at the point $x = x_m$ of local minimum of the function $U(x)$, does not vanish. In particular, the condition $\mathrm{E}(n) \ll 1$ may be fulfilled for all lower quantum numbers $n = 0, 1, 2, \ldots$ for smooth potentials of finite range l satisfying $\overline{h} \ll l\sqrt{2m|U_0|}$, with U_0 being the typical value of $U(x)$ (cf theorem 3 in section 5.1). This means that Planck's constant $\overline{h}$ should be small in comparison with the typical value of the classical action associated with the given potential well $U(x)$. On the other hand, in view of the strong singularity of the error-control integral at $k = 0$, caution should be used when applying the Bohr–Sommerfeld formula to the range of extremely small energies if the potential $U(x)$

vanishes at infinity, in spite of the fact that this range may correspond to large values of the Sommerfeld integral on the left-hand side of equation (4.99) and hence to large quantum numbers $n \gg 1$.

The equation (4.99) is *exact*. This is *not* the first-order quantization condition as obtained within the phase-integral method. The fact is that the term δ_n in the formula (4.99) stands for the *complete* sum of all higher-order correction terms which are obtainable in the phase-integral method. The estimate (4.100) pertains to this complete sum as a whole. What is done in the higher-order expansion scheme [12] may be regarded as extracting successive correction terms out of the quantity δ_n.

The estimate (4.100) is also *exact*. This means, first, that the relation (4.100) is valid for any potential $U(x)$ that is continuous and thrice continuously differentiable on the real axis. Secondly, the terms of all orders in powers of the error-control integral $\mathrm{E}(\nu)$ (3.89) are taken into account in the parameter $\varrho_n = \varrho_n(\varepsilon_n)$ (4.96) exactly. And, finally, there is no restriction upon the values of the phase integral $\int_a^b p(x)\,\mathrm{d}x$, neither on the left-hand side of the relation (4.99) nor in the quantity ϱ_n in the assessment (4.100).

Comparison with previous work. In [19, part B], Miller's [28] notation $U(b, x)$ and $\bar{U}(b, x)$ for the parabolic cylinder functions was used. The relation of the results obtained in the present paper, on the one hand, to those given in [19, part B], on the other hand, is established as follows. Functions used in [19, part B] are given on the left-hand sides of the formulae that follow, whereas corresponding quantities employed in the present work are written on the right-hand sides of those formulae, i.e.

$$\begin{gathered}
-u^2 f(u,a,x) \leftrightarrow p^2(x) \qquad g(u,a,x) = 0 \qquad \zeta\sqrt{u} \leftrightarrow \xi \qquad \alpha\sqrt{u} \leftrightarrow \xi_0 \\
b \leftrightarrow -\nu - \tfrac{1}{2} \qquad \rho(b) \leftrightarrow c_\nu \qquad \frac{1}{u}\psi(u,a,\zeta) \leftrightarrow (\xi')^2 R(x) \qquad \sqrt{\frac{\pi}{2}}\, l_1(b) \leftrightarrow \sigma_\nu \\
\frac{1}{\sqrt{2u}} V_{0,\zeta_2}(F) \leftrightarrow \mathrm{V}_+(0) \qquad \Omega(x) \leftrightarrow |\tfrac{1}{4}x^2 - \nu - \tfrac{1}{2}|^{1/2} \\
U(b,x) \leftrightarrow \left(\frac{2}{\pi}\right)^{1/4} \Gamma^{1/2}(\nu+1) w_\nu(x) \qquad \bar{U}(b,x) \leftrightarrow \left(\frac{2}{\pi}\right)^{1/4} \Gamma^{1/2}(\nu+1) u_\nu(x).
\end{gathered} \tag{7.124}$$

The connection formulae (2.5) are related to equations (5.9) in [19] through (7.124).

The Taylor series expansions (2.6) are new.

The uniform asymptotic forms (2.8) have been derived by the method of Langer [29], independently of those given in [22]. The equivalence of (2.8), on the one hand, and the formulae (5.12) and (5.13) in [19], on the other hand, may be verified by means of an appropriate change of variables.

The basic interval considered in the work [19] was the positive real axis $\zeta \geqslant 0$. For this reason, the auxiliary functions in [19, part B] were not defined for negative $\zeta < 0$. As a consequence, the statements, as well as the assessments (6.2) and (6.6), of the basic theorem I in [19] refer *only* to the positive real axis $\zeta \geqslant 0$.

The extension of the basic representations (2.10) to the negative real axis in section 2.2.2 is new, and so are the connection formulae (2.27) and (2.28) for the auxiliary functions $M_\nu(x)$ and $\theta_\nu(x)$.

On the *positive* real axis $\zeta \geqslant 0$, the auxiliary functions used in the two works are related by

$$\mathrm{M}(b,x) \leftrightarrow \left(\frac{2}{\pi}\right)^{1/4} \Gamma^{1/2}(\nu+1) M_\nu(x) \qquad \mathrm{N}(b,x) \leftrightarrow \left(\frac{2}{\pi}\right)^{1/4} \Gamma^{1/2}(\nu+1) N_\nu(x)$$
$$\mathrm{E}(b,x) \leftrightarrow E_\nu(x) \qquad \theta(b,x) \leftrightarrow \frac{\pi}{2} - \theta_\nu(x). \tag{7.125}$$

The uniform asymptotic representations (2.20)–(2.22), and (2.37), for the auxiliary functions are new.

The definition (2.23) for the basic parameter σ_ν, as well as its properties and its evaluation as a function of ν, are new. In particular, the parameter σ_ν is shown to be bounded in magnitude even in the limit $\nu \to +\infty$, while $\Omega(x) = O(x)$, unlike $l_1(b)$ given by equation (6.14) in [19]. Moreover, the limiting value σ_∞ (2.25) coincides with the number λ introduced in [10, p 397] relative to the Airy functions.

The definition and the properties of the parameter μ_ν in section 2.3 are new.

The definition of the amplitude function in section 2.4 is new.

For finite-range potentials $U(x)$ in quantum mechanics, the large parameter u in [19] may be identified with $k_0 l$ (5.107).

The explicit bounds (4.100) and (4.102) for the error term in the Bohr–Sommerfeld formula, in the case of two *distinct* real turning points, are sharper than the O-term in the formula of [19, section 6, p 162]. On the other hand, the results of [19] show that, through an appropriate choice of the function $\Omega(x)$, the estimate (4.100) may be made, under certain conditions, non-singular even in the limit $\nu \to -1/2$, when the two turning points coalesce.

In summary, the basic relations in the present work are simplified and extended, while the bounds are sharpened, with respect to those obtained in [19].

References

[1] Rajaraman R 1987 *Solitons and Instantons* (Amsterdam: North-Holland)
[2] Child M S 1991 *Semiclassical Mechanics with Molecular Applications* (Oxford: Clarendon)
[3] Kittel Charles 1986 *Introduction to Solid State Physics* (New York: Wiley)
[4] Hall R L 1995 *Phys. Rev.* A **51** 1787
[5] Buot F A 1993 *Phys. Rep.* **234** 73
[6] Hauge E H and Stovneng J A 1989 *Rev. Mod. Phys.* **61** 917
[7] Hauge E H, Falck J P and Fjeldly T A 1987 *Phys. Rev.* B **36** 4203
[8] Titchmarsh E C 1946 *Eigenfunction Expansions Associated with Second-order Differential Equations* (Oxford: Clarendon)
[9] Titchmarsh E C 1954 *Quart. J. Math. Oxford* **5** 228
[10] Olver F W J 1974 *Asymptotics and Special Functions* (New York: Academic)
[11] Kilpatrick J and Kilpatrick M 1948 *J. Chem. Phys.* **16** 781
[12] Lakshmanan M, Kaliappan P, Larsson K, Karlsson F and Fröman P O 1994 *Phys. Rev.* A **49** 3296
[13] Birkhoff G B 1933 *Bull. Am. Math. Soc.* **39** 696
[14] Kemble E C 1935 *Phys. Rev.* **48** 549
[15] Kemble E C 1958 *The Fundamental Principles of Quantum Mechanics* (New York: Dover)
[16] Heading J 1962 *An Introduction to Phase-Integral Methods* (London: Methuen)
[17] Fröman N and Fröman P O 1965 *JWKB Approximation* (Amsterdam: North-Holland)
[18] Moriguchi H 1959 *J. Phys. Soc. Japan* **14** 1771
[19] Olver F W J 1975 *Phil. Trans. R. Soc.* **278** 137
[20] Magnus W and Oberhettinger F 1948 *Formeln und Sätze für die Speziellen Funktionen der Mathematischen Physik* (Berlin: Springer)
[21] Erdélyi A, Kennedy M and McGregor J M 1954 *J. Rat. Mech. Anal.* **3** 459
[22] Olver F W J 1959 *J. Res. Nat. Bur. Standards* **63** B131
[23] Langer R E 1959 *Trans. Am. Math. Soc.* **90** 113

[24] Messiah A 1961 *Quantum Mechanics* (New York: Wiley)
[25] Chebotarev L V 1996 *J. Phys. A: Math. Gen.* **29** 1465
[26] Chebotarev L V 1995 *Phys. Rev.* A **52** 107
[27] Landau L D and Lifshitz E M 1977 *Quantum Mechanics* (Oxford: Pergamon)
[28] Miller J C P 1955 *Tables of Weber Parabolic Cylinder Functions* (London: HMSO)
[29] Langer R E 1932 *Trans. Am. Soc. Math.* **34** 447