Anharmonic Oscillator Equations: Treatment Parallel to Mathieu Equation

J.–Q. Liang\textsuperscript{a}\textsuperscript{*} and H. J.W. Müller-Kirsten\textsuperscript{b}\textsuperscript{†}

\textsuperscript{a)Institute of Theoretical Physics, Shanxi University, Taiyuan, Shanxi 030006, P.R. China}
\textsuperscript{b)Department of Physics, University of Kaiserslautern, D-67653 Kaiserslautern, Germany}

Abstract
The treatment of anharmonic oscillators (including double wells) by instanton methods is wellknown. The alternative differential equation method — excepting various WKB eigenvalue approximations — is not so wellknown. Here we reformulate the latter completely parallel to the strong coupling case of the cosine potential and Mathieu equation for which extensive literature and monographs exist. The solutions and eigenvalues of the anharmonic oscillator equations are obtained analogously as asymptotic expansions, and the exponentially small deviations are shown to follow from the imposition of boundary conditions — completely parallel to the case of the Mathieu equation. In spite of the additional involvement of WKB solutions, the exploitation of parameter symmetries of the basic equation (as in the case of the Mathieu equation) leads to a double well level splitting which agrees with the otherwise Furry–factor improved WKB approximation (and, of course, with calculations using periodic instantons).

1 Introduction
In a recent paper on new ways to solve the Schrödinger equation, R. Friedberg and T. D. Lee \textsuperscript{[1]} described the anharmonic oscillator case as a “long stand-

\textsuperscript{*}Email:jqliang@sxu.edu.cn
\textsuperscript{†}Email:mueller1@physik.uni-kl.de
ing difficult problem of a quartic potential with symmetric minima”. Quartic anharmonic oscillator potentials are for many reasons of fundamental interest in quantum mechanics and have therefore repeatedly been the subject of detailed investigations in diverse directions. In particular the investigations of Bender and Wu [2], [3] which related analyticity considerations to perturbation theory and hence to the large-order behaviour of the eigenvalue expansion attracted widespread interest. An important part of their work was concerned with the calculation of the imaginary part of the eigenenergy in the non-selfadjoint case which permits tunneling. Derivations of such a quantity are much less familiar than calculations of discrete bound state eigenenergies in quantum mechanical problems. This lack of popularity of the calculation of complex eigenvalues even in texts on quantum mechanics may be attributed to the necessity of matching various branches of eigenfunctions in domains of overlap and to the necessary imposition of suitable boundary conditions, both of which make the calculation more difficult.

The development and recognition of the significance of the path-integral method, particularly in connection with consideration of pseudo-particle configurations, displaced the Schrödinger equation into the shadow of the path-integral and suggested that little else would be gained from further studies of the differential equation. In addition, the equivalence of the two methods (at least in the one loop approximation) is not always appreciated [4].

Our intention in the following is to present treatment of the three different types of quartic anharmonic oscillators (these types arising from different signs of quadratic and quartic terms) formulated in parallel to the strong coupling case of the cosine potential [5], [6], the analogy with the periodicity of the latter entering only in the formulation of the boundary conditions. Indeed the Schrödinger equation with quartic oscillator potential should be raised to the rank of a standard differential equation akin to the Mathieu and similar equations which are not reducible to some hypergeometric type. Thus compare the equations

\[ y''(z) + [E - V(z)]y(z) = 0 \]

for \( V(z) = \begin{cases} 2h^2 \cos 2z = 2h^2 - 4h^2z^2 + \frac{4}{3}h^2z^4 \cdots & : \text{Mathieu}, \\ a^2 z^2 - b z^4 & : \text{quartic}. \end{cases} \]

Large-\( h^2 \) asymptotic expansions of the Mathieu equation are wellknown, and their lifting of the degeneracy of the asymptotically degenerate oscillator levels (i.e. for \( h^2 \to \infty \)) yields the boundaries of the energy bands obtained
with the (convergent) small-$\hbar^2$ expansion \[7,8\]. Books on Special Functions of Mathematical Physics contain all sorts of asymptotic expansions like the large-$\hbar^2$ expansion above, so that there is no reason to see in the allegedly "divergent perturbation series" of the anharmonic oscillator an ill-natured problem. These series are completely analogous to asymptotic expansions of Special Functions.

The treatment of the double-well potential by instanton methods and the calculation of its lowest level splitting \[9\] constitute a standard example of the path-integral method using instantons. The corresponding calculation for higher levels requires a different method \[10,11,12\] and is achieved with the use of periodic instantons \[13\] or other multi–instanton methods \[14\]. For the inverted double-well potential corresponding path-integral calculations using periodic instantons have been carried out in Ref. \[15\]. It is natural therefore to compare the Schrödinger and path-integral methods and it is reassuring to obtain in both cases identical results. Earlier WKB investigations of the eigenvalues of the Schrödinger equation with double well potential serve as valuable checks of the results of other methods, particularly since these have in some cases also been compared with numerical methods. However pure WKB results do not always agree with one-loop path-integral results \[9\]. Thus improved WKB approximations to double well eigenvalues have in particular been investigated and results in agreement with the instanton method have been achieved. Such WKB method investigations can be found particularly in Refs. \[16,17,18,19\] (regrettably with considerable suppression of intermediate steps).

In the following we review the method of the differential equation \[20\], however reformulated in parallel to the corresponding treatment of the Mathieu equation \[5\] for which the perturbation method in terms of a tunneling deviation from an integer (in the following $q - q_0, q_0 = 1, 3, 5, \ldots$) was originally developed. In our treatment here we leave various detailed calculational aspects to appendices. A feature different from that of the Mathieu equation is the additional involvement of WKB solutions for the evaluation of the boundary conditions at the central maximum in the case of the double well potential. However, exploiting parametric symmetries of the original Schrödinger equation, the level splitting obtained is in complete agreement with the Furry-factor corrected WKB result and that of the one-loop approximation in path-integral methods, the Furry-factor being a correction factor to the normalisation constant of the WKB wave function \[21\]. More detailed considerations are collected in our appendices which contain in addition to
calculational aspects, some WKB formulae for easy reference, since these are not always available but are essential in this context and are frequently or casually referred to as easily obtainable.

## 2 The Three Types of Potentials

In the cases treated most frequently in the literature the anharmonic oscillator potential is defined by the sum of an harmonic oscillator potential and a quartic contribution. These contributions may be given different signs, and thus lead to very different physical situations, which are nonetheless linked as a consequence of their common origin which is for all one and the same basic differential equation.

![](image)

**Fig. 1** The three different types of anharmonic potentials.

To avoid confusion we specify first the potential \( V(z) \) in the Schrödinger equation

\[
\frac{d^2 y(z)}{dz^2} + [E - V(z)]y(z) = 0
\]

for the different cases which are possible and illustrate these in Fig. 1. The three different cases are:

1. **Discrete eigenvalues with no tunneling**: In this case

   \[
   V(z) = \frac{1}{4}|h^4|z^2 + \frac{1}{2}|c^2|z^4,
   \]

2. **Discrete eigenvalues with tunneling**: In this case, described as the case
of the double well potential,

\[ V(z) = -\frac{1}{4}|h^4|z^2 + \frac{1}{2}|c^2|z^4, \]

(3) \textit{Complex eigenvalues with tunneling:} In this case, with the potential described as an inverted double well potential,

\[ V(z) = \frac{1}{4}|h^4|z^2 - \frac{1}{2}|c^2|z^4. \]

Case (1) is obviously the simplest with the anharmonic term implying simply a shift of the discrete harmonic oscillator eigenvalues with similarly normalisable wave functions. The shift of the eigenvalues is easily calculated with straightforward perturbation theory. The result is an expansion in descending powers of \( h^2 \). It is this expansion which led to a large number of investigations culminating (so to speak) in the work of Bender and Wu \cite{2,3} who established the asymptotic nature of the expansion* and its Borel summability.† The resulting eigenvalues are given by Eq. (34) below with \( q = q_0 = 2n + 1, n = 0, 1, 2, \ldots \) and \( c^2 \) replaced by \( -c^2 \), i.e.

\[ E(q, h^2) = \frac{1}{2}q_0h^2 + \frac{3c^2}{4h^4}(q_0^2 + 1) - \frac{c^4}{h^{10}}(4q_0^3 + 29q_0) + O\left(\frac{1}{h^{16}}\right). \]

Case (2) is also seen to allow only discrete eigenvalues (the potential rising to infinity on either side), however the central hump with troughs on either side permits tunneling and hence (if the hump is sufficiently high) a splitting of the asymptotically degenerate eigenvalues in the wells on either side which vanishes in the limit of an infinitely high central hump. The resulting eigenvalues are given by Eq. (145) below, i.e.

\[ E(q_0, h^2) \simeq E_0(q_0, h^2) \equiv \frac{2^{q_0 + 1}h^2(\frac{h^6}{2\pi})^{q_0/2}}{\sqrt{\pi}2^{q_0/4}[\frac{1}{2}(q_0 - 1)]!} e^{-\frac{h^6}{6\sqrt{2}c}}; \quad q_0 = 1, 3, 5, \ldots, \]

where \( E_0(q_0, h^2) \) is given by Eq. \cite{95} or Eq. \cite{C1}, i.e.

\[ E_0(q_0, h^2) = -\frac{h^8}{2^5c^2} + \frac{1}{\sqrt{2}}q_0h^2 - \frac{c^2(3q_0^2 + 1)}{2h^4} + O\left(\frac{1}{h^{10}}\right). \]

*This is shown by demonstrating that the \( i \)-th late term behaves like a factorial in \( i \) divided by an \( i \)-th power. See Ref. \cite{C2}.

†This is the case when the late terms alternate in sign.
Case (3) is seen to be very different from the first two cases, since the potential decreases without limit on either side of the centre. The boundary conditions are non-selfadjoint and hence the eigenvalues are complex. This type of potential allows tunneling through the barriers and hence a passage out to infinity so that a current can be defined. If the barriers are sufficiently high we expect the states in the trough to approximate those of an harmonic oscillator, however with decay as a consequence of tunneling. The resulting complex eigenvalues are given by Eq. (76) together with Eq. (34), i.e.

$$E = E_0(q_0, h^2) \left( -i \frac{2^{q_0} h^2 \left( \frac{h^6}{2 c^2} \right)^{q_0/2}}{(2\pi)^{1/2}(q_0 - 1)!} \right) e^{-\frac{h^6}{6c^2}}$$

with

$$E_0(q_0, h^2) = \frac{1}{2} q_0 h^2 - \frac{3c^2}{4h^2} (q_0^2 + 1) - \frac{c^4}{h^4} (4q_0^2 + 29q_0) + O\left( \frac{1}{h^{16}} \right).$$

The question is therefore: How does one calculate the eigenvalues in these cases with the help of the Schrödinger equation? This is the question we address here, and we present a fairly complete treatment of the case with large values of $h^2$ along lines parallel to those in the case of the cosine potential in Ref. [5]. We do not dwell on Case (1) since this is effectively included in the first part of Case (3), except for a change of sign of $|c^2|$. Thus we are mainly concerned with the double well potential and its inverted form.‡ We begin with the second. In this case our aim is to obtain the aforementioned complex eigenvalue. In the case of the double well potential our aim is to obtain the separation of harmonic oscillator eigenvalues as a result of tunneling between the two wells. Calculations of complex eigenvalues (imaginary parts of eigenenergies) are rare in texts on quantum mechanics. We therefore consider here in detail a prominent example and in such a way, that the general applicability of the method becomes evident.

‡In each of these two cases we have to take two different boundary conditions into account. In the cosine case of Ref. [3] only one type is required at $z = \pi/2$. The reason is that this is actually derived from the boundary condition at $z = 0$ using the periodicity of this case; see Ref. [7], equations (6), p. 108, and the relations (9), p. 100.
3 The Inverted Double–Well Potential

3.1 Defining the problem

We consider the case of the inverted double-well potential depicted as Case (3) in Fig. 1. The potential in this case is given by

\[ V(z) = -v(z), \quad v(z) = -\frac{1}{4} h^4 z^2 + \frac{1}{2} c^2 z^4, \]  

(1)

for \( h^4 \) and \( c^2 \) real and positive, and the Schrödinger equation to be considered is

\[ \frac{d^2 y}{dz^2} + [E + v(z)]y = 0. \]  

(2)

Fig. 2 The inverted double-well potential with (hatched) oscillator potential.

We adopt the following conventions which it is essential to state in order to assist comparison with other literature. We take \( \hbar = 1 \) and the mass \( m_0 \) of the particle = 1/2. This implies that results for \( m_0 = 1 \) (a frequent convention in field theory considerations) differ from those obtained here by factors of \( 2^{1/2} \), a point which has to be kept in mind in comparisons. If
suffixes 1/2, 1 refer to the two cases, we can pass from one to the other by making the replacements:

\[ E_{1/2} = 2E_1, \quad h^{4}_{1/2} = 2h^4_1, \quad c^2_{1/2} = 2c^2_1. \]  

(3)

Introducing a parameter \( q \) and a quantity \( \Delta \equiv \Delta(q, h) \), and a variable \( w \) defined by setting

\[ E = \frac{1}{2}qh^2 + \frac{\Delta}{2h^4} \quad \text{and} \quad w = hz, \]  

(4)

we can rewrite Eq. (2) as

\[ D_q(w)y(w) = -\frac{1}{h^8}(\Delta + c^2w^4)y(w) \]  

(5)

with

\[ D_q(w) = 2\frac{d^2}{dw^2} + q - \frac{w^2}{2}. \]  

(6)

In the domain of \( w \) finite, \(|h^2| \to \infty\) and \( c^2 \) finite, the harmonic part of the potential dominates over the quartic contribution and Eq. (5) becomes

\[ D_q(w)y(w) = O\left(\frac{1}{h^2}\right). \]  

(7a)

The problem then reduces to that of the pure harmonic oscillator with \( y(w) \) a parabolic cylinder function, i.e.

\[ y(w) \propto D_{\frac{1}{2}(q-1)}(w) \quad \text{and} \quad q = q_0 = 2n + 1, \quad n = 0, 1, 2, \ldots. \]  

(7b)

The perturbation expansion in descending powers of \( h \) suggested by the above considerations is therefore an expansion around the central minimum of \( V(z) \) at \( z = 0 \). The positions \( z_{\pm} \) of the maxima of \( V(z) \) on either side of \( z = 0 \) in the case \( c^2 > 0 \) are obtained from

\[ v'(z_\pm) = 0 \quad \text{as} \quad z_{\pm} = \pm \frac{h^2}{2c} \]  

(8)

with

\[ v''(z_\pm) = h^4 \quad \text{and} \quad V(z_{\pm}) = \frac{h^8}{2^9c^2}. \]
Thus for $c^2 > 0$ and relatively small, and $h^2$ large the eigenvalues are essentially perturbatively shifted eigenvalues of the harmonic oscillator as is evident from Fig. 1.

The problem here is to obtain the solutions in various domains of the variable, to match these in domains of overlap, then to specify the necessary boundary conditions and finally to exploit the latter for the derivation of the complex eigenvalue. The result will be that derived originally by Bender and Wu [2], [3], although our method here (which parallels that used in the case of the cosine potential) is different.

### 3.2 Three pairs of solutions

We are concerned with the equation

$$\frac{d^2y(z)}{dz^2} + \left[ E - \frac{h^4z^2}{4} + \frac{c^2z^4}{2} \right] y(z) = 0 \quad (9)$$

where

$$E = \frac{1}{2} qh^2 + \frac{\Delta}{2h^4}. \quad (10)$$

Here again $q$ is a parameter still to be determined from boundary conditions, and $\Delta = \Delta(q, h)$ is obtained from the perturbation expansion of the eigenvalue, as encountered and explained earlier. Inserting (10) into (9) we obtain

$$\frac{d^2y}{dz^2} + \left[ \frac{1}{2} qh^2 + \frac{\Delta}{2h^4} - \frac{h^4z^2}{4} + \frac{c^2z^4}{2} \right] y = 0. \quad (11)$$

The solutions in terms of parabolic cylinder functions are valid around $z = 0$ and extend up to $z \simeq O(1/h^2)$, as we shall see. Before we return to these solutions we derive a new pair which is valid in the adjoining domains. Thus these solutions are not valid around $z = 0$. In order to arrive at these solutions we set in Eq. (11)

$$y(z) = A(z) \exp \left[ \pm i \int z dz \left\{ - \frac{h^4z^2}{4} + \frac{c^2z^4}{2} \right\}^{1/2} \right]. \quad (12)$$

Then $A(z)$ is found to satisfy the following equation

$$A''(z) \pm 2i \left\{ - \frac{h^4z^2}{4} + \frac{c^2z^4}{2} \right\}^{1/2} A'(z) \pm iA(z) \frac{d}{dz} \left\{ - \frac{h^4z^2}{4} + \frac{c^2z^4}{2} \right\}^{1/2}$$

$$+ \left[ \frac{1}{2} qh^2 + \frac{\Delta}{2h^4} \right] A(z) = 0. \quad (13)$$
Later we will be interested in the construction of wave functions which are even or odd around $z = 0$. This construction is simplified by the consideration of symmetry properties of our solutions which arise at this point. We observe — before touching the square roots in Eq. (13) — that one equation (of the two alternatives) follows from the other by changing the sign of $z$ throughout. This observation allows us to define the pair of solutions

$$y_A(z) = A(z) \exp \left[ + i \int^z \! dz \left\{ - \frac{h^4 z^2}{4} + \frac{c^2 z^4}{2} \right\}^{1/2} \right], \quad (14a)$$

$$\bar{y}_A(z) = \overline{A}(z) \exp \left[ - i \int^z \! dz \left\{ - \frac{h^4 z^2}{4} + \frac{c^2 z^4}{2} \right\}^{1/2} \right], \quad (14b)$$

with

$$\overline{A}(z) = A(-z) \quad \text{and} \quad \overline{y}_A(z) = y_A(-z), \quad (15)$$

where $A(z)$ is the solution of the upper of Eqs. (13) and $\overline{A}(z)$ that of the lower of these equations. We take the square root by setting

$$\left\{ - \frac{z^2 h^4}{4} \right\}^{1/2} = (-i) \frac{z h^2}{2}. \quad (16)$$

For large $h^2$ we can write the Eqs. (13) as

$$\mp z A'(z) + \frac{1}{2} A(z) + \frac{1}{2} q A(z) = O \left( \frac{1}{h^2} \right).$$

We define $A_q(z)$ as the solution of the equation

$$z A'_q(z) - \frac{1}{2} (q - 1) A_q(z) = 0, \quad (17)$$

i.e.

$$A_q(z) = z^{\frac{1}{2}(q-1)} \equiv \frac{1}{(z^2)^{1/4}} \exp \left[ \frac{1}{2} q \int^z \! \frac{dz}{(z^2)^{1/2}} \right]. \quad (18)$$

We define correspondingly

$$\overline{A}_q(z) = z^{-\frac{1}{2}(q+1)} = A_{-q}(z) \equiv \frac{1}{(z^2)^{1/4}} \exp \left[ - \frac{1}{2} q \int^z \! \frac{dz}{(z^2)^{1/2}} \right]. \quad (19)$$

We see that one solution follows from the other by replacing $z$ by $-z$. Clearly $A_q(z), \overline{A}_q(z)$ approximate the solutions of Eqs. (13) and we can develop a
perturbation theory along the lines of our method as employed in the case of periodic potentials. One finds that these solutions are associated with the same asymptotic expansion for $\Delta$ — to be derived in detail below in Appendix A and as a verification again in connection with the solution $y_B$ — as the other solutions. Since these higher order contributions are of little interest for our present considerations, we do not pursue their calculation. Thus we now have the pair of solutions

$$y_A(z) = \exp \left[ i \int^z dz \left\{ -\frac{1}{4} z^2 h^4 + \frac{1}{2} c^2 z^4 \right\}^{1/2} \right] A_q(z) + O(\frac{1}{h^2}), \quad (20a)$$

$$\overline{y}_A(z) = \exp \left[ -i \int^z dz \left\{ -\frac{1}{4} z^2 h^4 + \frac{1}{2} c^2 z^4 \right\}^{1/2} \right] \overline{A}_q(z) + O(\frac{1}{h^2}). \quad (20b)$$

These expansions are valid as decreasing asymptotic expansions in the domain

$$|z| > O\left(\frac{1}{h}\right),$$

i.e. away from the central minimum. With proper care in selecting signs of square roots we can use the solutions \textit{(20a)} and \textit{(20b)} to construct solutions $y_\pm(z)$ which are respectively even and odd under the parity transformation $z \to -z$ (or equivalently $q \to -q, h^2 \to -h^2$), i.e. we write

$$y_\pm(z) = \frac{1}{2} [y_A(q, h^2, z) \pm \overline{y}_A(q, h^2, z)]. \quad (21)$$

In the next two pairs of solutions the exponential factor of the above solutions of type $A$ is contained in the parabolic cylinder functions (which are effectively exponentials times Hermite functions).

We return to Eq. \textit{(5)}. The solutions $y_q(z)$ of the equation

$$D_q(w)y_q(w) = 0, \quad w = hz, \quad (22)$$

are parabolic cylinder functions $D_{\frac{1}{2}(q-1)}(\pm w)$ and $D_{-\frac{1}{2}(q+1)}(\pm iw)$ (observe that Eq. \textit{(22)} is invariant under the combined substitutions $q \to -q, w \to \pm iw$) or functions

$$B_q(w) = \frac{D_{\frac{1}{2}(q-1)}(\pm w)}{[\frac{1}{2}(q-1)]! 2^{\frac{1}{2}(q-1)}} \quad \text{and} \quad C_q(w) = \frac{D_{-\frac{1}{2}(q+1)}(\pm iw) 2^{\frac{1}{2}(q+1)}}{[-\frac{1}{2}(q+1)]!}. \quad (23)$$
These solutions satisfy the following recurrence relation (obtained from the basic recurrence relation for parabolic cylinder functions given in the literature\footnote{Ref. \cite{23}, pp. 115 - 123. Comparison with our notation is easier if this reference is used.})

\[ w^2 y_q = \frac{1}{2} (q + 3) y_{q+4} + q y_q + \frac{1}{2} (q - 3) y_{q-4}. \]  

(24)

The extra factors in Eq. (23) have been inserted to make this recurrence relation assume this particularly symmetric and appealing form.\footnote{As an alternative to \( B_q(w) \) in Eq. (23) one can choose the solutions as \( \tilde{B}_q(w) \) with

\[ \tilde{B}_q(w) = \frac{D_{4q-1}(w)}{[\frac{1}{2} (q - 3)]^{2q+1}.} \]

These satisfy the recurrence relation

\[ w^2 y_q(w) = \frac{1}{2} (q + 1) y_{q+4} + q y_q + \frac{1}{2} (q - 1) y_{q-4}. \]}

For higher even powers of \( w \) we write

\[ w^{2i} y_q = \sum_{j=-i}^{i} S_{2i}(q, 4j) y_{q+4j}, \]  

(25)

where in the case \( i = 2 \)

\[ S_4(q, \pm 8) = \frac{1}{4} (q \pm 3)(q \pm 7), \]

\[ S_4(q, \pm 4) = (q \pm 2)(q \pm 3), \]

\[ S_4(q, 0) = \frac{3}{2} (q^2 + 1). \]  

(26)

The first approximation \( y(w) = y^{(0)}(w) = y_q(w) \) therefore leaves uncompensated terms amounting to

\[ P_q^{(0)} = -\frac{1}{\hbar^6} (\triangle + c^2 w^4) y_q(w) \equiv -\frac{1}{\hbar^6} \sum_{j=-2}^{2} [q, q + 4j] y_{q+4j}, \]  

(27)

where

\[ [q, q] = \triangle + c^2 S_4(q, 0), \]  

and for \( j \neq 0 : \]

\[ [q, q + 4j] = c^2 S_4(q, 4j). \]  

(28)
Now, since \( D_q y_q = 0 \), we also have \( D_{q+4j} y_{q+4j} = 0 \), and so
\[
D_q y_{q+4j}(w) = -4j y_{q+4j}(w).
\] (29)

Hence a term \( \mu y_{q+4j} \) on the right hand side of Eq. (27) can be removed by adding to \( y^{(0)} \) the contribution \( (-\mu/4j)y_{q+4j} \). Thus the next order contribution to \( y_q \) is
\[
y^{(1)}(w) = \frac{1}{h^6} \sum_{j=-2,j\neq0}^{2} \frac{[q, q + 4j]}{4j} y_{q+4j}.
\] (30)

For the sum \( y(w) = y^{(0)}(w) + y^{(1)}(w) \) to be a solution to that order we must also have to that order
\[
[q, q] = 0, \quad \text{i.e.} \quad \triangle = -\frac{3}{2}(q^2 + 1)c^2 + O\left(\frac{1}{h^6}\right). \quad (31)
\]

Proceeding in this way we obtain the solution
\[
y = y^{(0)}(w) + y^{(1)}(w) + y^{(2)}(w) + \cdots
\] (32)

with the corresponding equation from which \( \triangle \) can be obtained, i.e.
\[
0 = \frac{1}{h^6} [q, q] + \left(\frac{1}{h^6}\right)^2 \sum_{j \neq 0} [q, q + 4j]\frac{[q + 4j, q]}{4j} + \cdots \quad (33)
\]

Evaluating this expansion and inserting the result for \( \triangle \) into Eq. (10) we obtain
\[
E(q, h^2) = \frac{1}{2} qh^2 - \frac{3c^2}{4h^4}(q^2 + 1) - \frac{c^4}{h^10}(4q^3 + 29q) + O\left(\frac{1}{h^16}\right). \quad (34)
\]
We observe that odd powers of \( q \) arise in combination with odd powers of \( 1/h^2 \), and even powers of \( q \) in combination with even powers of \( 1/h^2 \), so that the entire expansion is invariant under the interchanges
\[
q \rightarrow -q, \quad h^2 \rightarrow -h^2.
\]

This type of invariance is a property of a very large class of eigenvalue problems. Equation (34) is the expansion of the eigenenergies \( E \) of Case (1) with \( q = q_0 = 2n + 1, n = 0, 1, 2, \ldots \). In Case (3) the parameter \( q \) is only approximately an odd integer, the difference \( q - q_0 \) arising from tunneling..
We can now write the solution $y(w)$ in the form

$$y(w) = y_q(w) + \sum_{i=1}^{\infty} \left( \frac{1}{h^6} \right)^i \sum_{j=-2i,j\neq0}^{2i} P_i(q, q + 4j)y_{q+4j}(w), \quad (35)$$

where for instance

$$P_1(q, q \pm 4) = \left[ q, q \pm 4 \right]_{\pm4} = c^2 \frac{(q \pm 2)(q \pm 3)}{\pm4},$$

$$P_2(q, q \pm 4) = \left[ q, q \pm 4 \right]_{\pm4} \left[ q \pm 4, q \pm 4 \right]_{\mp4} + \frac{[q, q \pm 4] [q \pm 8, q \pm 4]}{\pm8},$$

and so on. Again we can write down a recurrence relation for the coefficients $P_i(q, q + 4j)$, i.e.

$$4tP_i(q, q + 4t) = \sum_{j=-2}^{2} P_{i-1}(q, q + 4j + 4t)[q + 4j + 4t, q + 4t] \quad (36)$$

with the boundary conditions

$$P_0(q, q) = 1, \quad \text{and for } j \neq 0 \text{ all other } P_0(q, q + 4j) = 0,$$

$$P_{i\neq0}(q, q) = 0,$$

$$P_i(q, q + 4j) = 0 \text{ for } |j| > 2i \text{ or } |j| \geq 2i + 1. \quad (37)$$

For further details concerning these coefficients, their recurrence relations and the solutions of the latter we refer to Ref. [20]. Since our starting equation is invariant under a change of sign of $z$, we may infer that given one solution $y(z)$, there is another solution $y(-z)$. We thus have the following pair of solutions

$$y_B(z) = \left[ B_q(w) + \sum_{i=1}^{\infty} \left( \frac{1}{h^6} \right)^i \sum_{j=-2i,j\neq0}^{2i} P_i(q, q + 4j)B_{q+4j}(w) \right]_{w=hz, \arg z=0},$$

$$\bar{y}_B(z) = [y_B(z)]_{\arg z=\pi} = [y_B(-z)]_{\arg z=0}. \quad (38)$$

These solutions are suitable in the sense of decreasing asymptotic expansions in the domains

$$|z| \lesssim O\left( \frac{1}{h^2} \right), \quad \arg z \sim 0, \pi.$$
They are linearly independent there as long as \( q \) is not an integer.

Our third pair of solutions is obtained from the parabolic cylinder functions of complex argument. We observed earlier that these are obtained by making the replacements

\[
q \to -q, \quad w \to \pm iw.
\]

These solutions are therefore defined by the following substitutions:

\[
y_C(z) = [y_B(z)]_{q \to -q, \ h \to ih}, \quad \overline{y}_C(z) = [\overline{y}_B(z)]_{q \to -q, \ h \to ih}
\]

with the same coefficients \( P_i(q, q + 4) \) as in \( y_B \). The solutions \( y_C, \overline{y}_C \) are suitable asymptotically decreasing expansions in one of the domains

\[
|z| \lesssim O\left(\frac{1}{h^2}\right), \quad \arg z \sim \pm \frac{\pi}{2}.
\]

We emphasise again that all three pairs of solutions are associated with the same expansion of the eigenvalue \( E(q, h^2) \) in which odd powers of \( q \) are associated with odd powers of \( h^2 \), so that the eigenvalue expansion remains unaffected by the interchanges \( q \to -q, \ h^2 \to -h^2 \) as long as corrections resulting from boundary conditions are ignored.

### 3.3 Matching of solutions

We saw that the solutions of types \( B \) and \( C \) are valid around the central minimum at \( |z| = 0 \), the solutions of type \( A \) being valid away from the minimum. Thus in the transition region some become proportional. In order to be able to extract the proportionality factor between two solutions, one has to stretch each by appropriate expansion to the limit of its domain of validity. In this bordering domain the adjoining branches of the overall solution then differ by a constant.\(^{\text{II}}\)

First we deal with the exponential factor in the solutions of type \( A \). Since these are not valid around \( z = 0 \) but \( h^2 \) is assumed to be large, we expand

\(^{\text{II}}\)Variables like those we use here for expansion about the minimum of a potential (e.g. like \( w \) of Eq. (4)) are known in some mathematical literature as “stretching variables” and are there discussed in connection with matching principles, see e.g. Ref. [24].
the integrand as follows:

\[
\exp \left[ i \int dz \left\{ -\frac{1}{4} z^2 h^4 + \frac{1}{2} c^2 z^4 \right\}^{1/2} \right] 
= \exp \left[ \frac{h}{8c^2} \int dz \left( \frac{2c^2 z^2}{h^4} \right) \left\{ 1 - \frac{2c^2 z^7}{h^4} \right\} \right] 
= \exp \left[ \frac{h}{12c^2} - \frac{h^2 z^2}{4} + O \left( \frac{z^4}{h^2} \right) \right].
\]

(40)

Considering the pair of solutions \( y_A(z), y_A(z) \) we see that in the direction of \( z = 0 \) (of course, not around that point)

\[
y_A(z) = e^{h^6/12c^2} e^{-1/4 z^2 h^2} \left[ z^{1/2(q-1)} + O \left( \frac{1}{h^2} \right) \right],
\]

\[
y_A(z) = e^{-h^6/12c^2} e^{1/4 z^2 h^2} \left[ z^{-1/2(q+1)} + O \left( \frac{1}{h^2} \right) \right].
\]

(41)

The cases of the solutions of types \( B \) and \( C \) require a careful look at the parabolic cylinder functions since these differ in different regions of the argument of the variable \( z \). Thus from the literature [25] we obtain

\[
D_{\frac{1}{2}(q-1)}(w) = w^{\frac{1}{2}(q-1)} e^{-\frac{1}{4} w^2} \sum_{i=0}^{\infty} \frac{\left[ \frac{1}{2}(q-1) \right]!}{i! \left[ \frac{1}{2}(q-4i-1) \right]! (-2w^2)^i}, \quad |\arg w| < \frac{3}{4},
\]

but

\[
D_{\frac{1}{2}(q-1)}(w) = w^{\frac{1}{2}(q-1)} e^{-\frac{1}{4} w^2} \sum_{i=0}^{\infty} \frac{\left[ \frac{1}{2}(q-1) \right]!}{i! \left[ \frac{1}{2}(q-4i-1) \right]! (-2w^2)^i} - \frac{(2\pi)^{1/2} e^{-i\pi/2(q-1)}}{w^{1/2(q+1)}} \sum_{i=0}^{\infty} \frac{\left[ -\frac{1}{2}(q+1) \right]!}{i! \left[ -\frac{1}{2}(q+4i+1) \right]! (2w^2)^i}
\]

with \( \frac{5}{4} > \arg w > \frac{1}{4} \).

(42)

The function \( D_{\frac{1}{2}(q-1)}(w) \) has a similarly complicated expansion for

\[-\frac{1}{4} > \arg w > -\frac{5}{4} \].

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From (42) we obtain for the solution \( y_B(z), w = hz \):

\[
y_B(z) \simeq B_q(w) = \frac{(h^2 z^2)^{\frac{1}{4}(q-1)}}{[\frac{1}{4}(q-1)]!2^{\frac{1}{4}(q-1)}} e^{-\frac{1}{4}h^2 z^2} \left[ 1 + O\left(\frac{1}{h^2}\right) \right]. \tag{44}
\]

In the solution \( \overline{y}_B(z) \), with \( z \) in \( y_B(z) \) replaced by \(-z\), we would have to substitute correspondingly the expression (43) (since \( z \to -z \) implies \( \arg z = \pm \pi \)). We do not require this at present. Comparing the solution \( y_A(z) \) of Eq. (41) with the solution \( y_B(z) \) of Eq. (44) we see that in their common domain of validity

\[
y_A(z) = \frac{1}{\alpha} y_B(z) \tag{45}
\]

with

\[
\alpha = \frac{(h^2)^{\frac{1}{4}(q-1)} e^{-\frac{h^6}{12c^2}}}{[\frac{1}{4}(q-1)]!2^{\frac{1}{4}(q-1)}} \left[ 1 + O\left(\frac{1}{h^2}\right) \right]. \tag{46}
\]

However, the ratio of \( \overline{y}_A(z), \overline{y}_B(z) \) is not a constant.

We proceed similarly with the solutions \( y_C(z), \overline{y}_C(z) \). Inserting the expansion (42) into \( \overline{y}_C(z) \) we obtain

\[
\overline{y}_C(z) = \frac{(-h^2 z^2)^{\frac{1}{2}(q+1)} e^{\frac{h^6}{12c^2} z^2}}{[-\frac{1}{4}(q+1)]!2^{\frac{1}{4}(q+1)}} \left[ 1 + O\left(\frac{1}{h^2}\right) \right]. \tag{47}
\]

Comparing this behaviour of the solution \( \overline{y}_C(z) \) with that of solution \( \overline{y}_A(z) \) of Eq. (11), we see that in their common domain of validity

\[
\overline{y}_A(z) = \frac{1}{\overline{\alpha}} \overline{y}_C(z), \tag{48}
\]

where

\[
\overline{\alpha} = \frac{(-h^2)^{\frac{1}{4}(q+1)} e^{\frac{h^6}{12c^2}}}{[-\frac{1}{4}(q+1)]!2^{-\frac{1}{4}(q+1)}} \left[ 1 + O\left(\frac{1}{h^2}\right) \right]. \tag{49}
\]

Again there is no such simple relation between \( y_A(z) \) and \( y_C(z) \).

### 3.4 Boundary conditions at the origin

(A) Formulation of the boundary conditions

The really difficult part of the problem is to recognise the boundary conditions we have to impose. Looking at the potential we are considering here
— as depicted in Fig. 2 — we see that near the origin the potential behaves like that of the harmonic oscillator, in fact, our large-$h^2$ solutions require this for large $h^2$. Thus the boundary conditions to be imposed there are the same as in the case of the harmonic oscillator for alternately even and odd wave functions. Recalling the solutions $y_{\pm}(z)$ which we defined with Eq. (21) as even and odd about $z = 0$, we see that at the origin we have to demand the conditions

$$y_+(0) = 0 \quad \text{and} \quad y_-(0) = 0$$

and $y_+(0) \neq 0, y'_+(0) \neq 0$. The first of the conditions will be seen to imply $q_0 \equiv 2n + 1 = 1, 5, 9, \ldots$ and the second $q_0 = 3, 7, 11, \ldots$. For instance $q_0 = 1$ (or $n = 0$) implies a ground state wave function with the shape of a Gauss curve above $z = 0$, i.e. large probability for the particle to be found thereabouts. At $z = 0$ the solutions of type $A$ are invalid; hence we have to use the proportionality just derived in order to match these to the solutions valid around the origin. Then imposing the above boundary conditions we obtain

$$0 = y'_+(0) = \lim_{z \to 0} \frac{1}{2} [y'_A(z) + \overline{y}_A(z)]$$

$$= \frac{1}{2} \left[ \frac{1}{\alpha} y'_B(0) + \frac{1}{\alpha} \overline{y}_C(0) \right]$$

and

$$0 = y_-(0) = \lim_{z \to 0} \frac{1}{2} [y_A(z) - \overline{y}_A(z)]$$

$$= \frac{1}{2} \left[ \frac{1}{\alpha} y_B(0) - \frac{1}{\alpha} \overline{y}_C(0) \right].$$

Thus we obtain the equations

$$\frac{y'_B(0)}{\overline{y}_C(0)} = -\frac{\alpha}{\overline{\alpha}} \quad \text{and} \quad \frac{y_B(0)}{\overline{y}_C(0)} = \frac{\alpha}{\overline{\alpha}}.$$  

Clearly we now have to evaluate the solutions involved and their derivatives at the origin. We leave details to Appendix B.

(B) Evaluation of the boundary conditions

We now evaluate Eqs. (53) in dominant order and insert from Eqs. (46), (49) the appropriate expressions for $\alpha$ and $\overline{\alpha}$. Starting with the derivative
expression we obtain (apart from contributions of order \(1/h^2\))

\[
-\frac{1}{i} \sin \left\{ \frac{\pi}{4} (q + 3) \right\} - \frac{\pi^2}{i} \sin \left\{ \frac{\pi}{4} (q - 3) \right\} = \frac{(h^2)^{\frac{1}{2}(q-1)} \left[ -\frac{1}{4} (q + 1) \right]! 2^{-\frac{1}{2}(q+1)}}{\left[ \frac{1}{4} (q - 1) \right]! 2^{\frac{1}{2}(q-1)} (-h^2)^{-\frac{1}{2}(q+1)}} e^{-\frac{h^6}{6c^2}}.
\]

We rewrite the left hand side as

\[
-\frac{i}{\sin \left\{ \frac{\pi}{4} (q + 3 - 6) \right\} = i \tan \left\{ \frac{\pi}{4} (q + 3) \right\}.
\]

We rewrite the right hand side of the derivative equation again with the help of the inversion and duplication formulae and obtain

\[
\pi \left( \frac{h^4}{4} \right)^{q/4} (-1)^{q+1} e^{-h^6/6c^2} \left[ \frac{1}{4} (q - 1) \right]! \left[ \frac{1}{4} (q - 3) \right]! \sin \left\{ \frac{\pi}{4} (q + 1) \right\} = \sqrt{2} \left[ \frac{1}{2} (q - 1) \right]! \cos \left\{ \frac{\pi}{4} (q + 3) \right\} e^{-\frac{h^6}{6c^2}}.
\]

Then the derivative relation of (53) becomes

\[
\sin \left\{ \frac{\pi}{4} (q + 3) \right\} = -i \sqrt{\frac{\pi}{2}} \left( \frac{h^4}{4} \right)^{q/4} (-1)^{q+1} e^{-\frac{h^6}{6c^2}}.
\]

Proceeding similarly with the second of relations (53), we obtain

\[
\cos \left\{ \frac{\pi}{4} (q + 3) \right\} = -\sqrt{\frac{\pi}{2}} \left( \frac{h^4}{4} \right)^{q/4} (-1)^{q+1} e^{-\frac{h^6}{6c^2}}.
\]

In each of Eqs. (54) and (55) the right hand side is an exponentially small quantity. In fact the left hand side of (54) vanishes for \(q = q_0 = 1, 5, 9, \ldots\) and the left hand side of (55) for \(q = q_0 = 3, 7, 11, \ldots\). With a Taylor expansion about \(q_0\) the left hand side of (54) becomes

\[
(q - q_0) \frac{\pi}{4} \cos \left\{ \frac{\pi}{4} (q + 3) \right\} + \cdots \simeq (q - q_0) \frac{\pi}{4} (-1)^{-\frac{1}{2}(q_0+3)}.
\]

It follows that we obtain for the even function with \(q = q_0 = 1, 5, 9, \ldots\)

\[
(q - q_0) \simeq \pm \frac{2\sqrt{2}}{\sqrt{\pi}} \frac{(h^2)^{q_0/2}}{\left[ \frac{1}{2} (q_0 - 1) \right]!} e^{-\frac{h^6}{6c^2}}.
\]

Expanding similarly the left hand side of Eq. (55) about \(q_0 = 3, 7, 11, \ldots\), we again obtain (56) but now for the odd function with these values of \(q_0\). We have thus obtained the conditions resulting from the boundary conditions at \(z = 0\). Our next task is to extend the solution all the way to the region beyond the shoulders of the inverted double well potential and to impose the necessary boundary conditions there. Thus we have to determine these conditions first.
3.5 Boundary conditions at infinity

(A) Formulation of the boundary conditions

We explore first the conditions we have to impose at $|z| \to \infty$. Recall the original Schrödinger equation (2) with potential (1). For $c^2 < 0$ and the solution $y(z)$ square integrable in $-\infty < \Re z < \infty$, the energy $E$ is real; this is the case of the purely discrete spectrum (the differential operator being selfadjoint for the appropriate boundary conditions, i.e. the vanishing of the wave functions at infinity). This is Case (1) of Fig. 1. The analytic continuation of one case to the other is accomplished by replacing $\pm c^2$ by $\mp c^2$ or, equivalently, by the rotations

$$E \to e^{i\pi} E = -E, \quad z \to e^{i\pi/2} z, \quad z^2 \to -z^2.$$  

One can therefore retain $c^2$ as it is and perform these rotations. It is then necessary to insure that when one rotates to the case of the purely discrete spectrum without tunneling, the resulting wave functions vanish at infinity and thus are square integrable. Thus in our case here the behaviour of the solutions at infinity has to be chosen such that this condition is satisfied. Now, for $\Re z \to \pm \infty$ we have

$$y(z) \sim \exp \left\{ \pm i \int z \left[ \frac{c^2}{2} z^4 \right]^{1/2} \right\} = \exp \left\{ \pm i \left( \frac{c^2}{2} \right)^{1/2} \left| z \right|^3 \right\}. \quad (57)$$

In order to decide which solution or combination of solutions is compatible with the square integrability in the rotated ($c^2$ reversed) case, we set

$$z = |z| e^{i\theta}.$$  

Then

$$\exp \left\{ -i \left( \frac{c^2}{2} \right)^{1/2} \left| z \right|^3 \right\} = \exp \left\{ -i \left( \frac{c^2}{2} \right)^{1/2} \left| z \right|^3 e^{3i\theta} \right\}$$

$$= \exp \left\{ -i \left( \frac{c^2}{2} \right)^{1/2} \left| z \right|^3 \left( \cos 3\theta + i \sin 3\theta \right) \right\}$$

$$\propto \exp \left\{ \left( \frac{c^2}{2} \right)^{1/2} \left| z \right|^3 \sin 3\theta \right\}.$$
This expression vanishes for $|z| \to +\infty$ if the angle $\theta$ lies in the range $-\pi < 3\theta < 0$, i.e. if $-\pi/3 < \theta < 0$. Thus

$$\exp \left\{ -i \left( \frac{c^2}{2} \right)^{1/2} \frac{z^3}{3} \right\} \to 0 \quad \text{for } \Re z \to +\infty \quad \text{in } \arg z \in \left( -\frac{\pi}{3}, 0 \right),$$

$$\exp \left\{ +i \left( \frac{c^2}{2} \right)^{1/2} \frac{z^3}{3} \right\} \to 0 \quad \text{for } \Re z \to -\infty \quad \text{in } \arg z \in \left( 0, \frac{\pi}{3} \right). \quad (58)$$

Rotating $z$ by $\pi/2$, i.e. replacing $\sin 3\theta$ by $\sin 3\left( \theta + \frac{\pi}{2} \right) = -\cos 3\theta$

we see that the solution with the exponential factor is exponentially decreasing for $|z| \to \infty$ provided that

$$\cos 3\theta > 0,$$

i.e. in the domain $-\pi/2 < 3\theta < \pi/2$, or

$$-\frac{\pi}{6} < \theta < \frac{\pi}{6}.$$

In the case of the inverted double well potential under consideration here (i.e. the case of complex $E$), we therefore demand that for $\Re z \to +\infty$ and $-\pi/3 < \arg z < 0$ the wave functions have decreasing phase, i.e.

$$y(z) \sim \exp \left\{ -i \left( \frac{c^2}{2} \right)^{1/2} \frac{z^3}{3} \right\}, \quad c^2 > 0. \quad (59)$$

This is the boundary condition also used by Bender and Wu [2]. For $c^2 < 0$ we have correspondingly

$$y(z) \sim \exp \left\{ \pm \left( \frac{|c^2|}{2} \right)^{1/2} \frac{z^3}{3} \right\}, \quad c^2 < 0, \quad \text{for } z \to \mp \infty.$$

This is not the asymptotic behaviour of a wave function of the simple harmonic oscillator. We have to remember that we have various branches of the solutions $y(z)$ in different domains of $z$.

Our procedure now is to continue (in the sense of matched asymptotic expansions) the even and odd solutions (21) to $+\infty$ and to demand that
they satisfy the condition (59) for $c^2 > 0$. Equating to zero the coefficient of the term with sign opposite to that in the exponential of Eq. (59) will lead to our second condition which together with the first obtained from boundary conditions at the origin determines the imaginary part of the eigenvalue $E$.

![Fig. 3 The inverted double-well potential with turning points $z_0, z_1$.](image)

(B) Evaluation of the boundary conditions

The following considerations (usually for real $z$) require some algebraic steps which could obscure the basic procedure. We therefore explain our procedure first. Our even and odd solutions $y_{\pm}(z)$ (cf. Eq. (21)) were defined in terms of solutions of type $A$ which have a wide domain of validity. Looking at Fig. 3 we see that at a given energy $E$ and to the right of $z = 0$ (which is the only region we consider for reasons of symmetry) there are two turning points $z_0, z_1$. Thus we have to match the solutions of type $A$ first to solutions to the left of $z_1$ and then extend these to solutions to the right, and there impose the boundary condition (59) on $y_{\pm}(z)$ (by demanding that the coefficient of the solutions with other behaviour be zero). We do this extension with the help of WKB solutions, i.e. we match the WKB solutions to the left of $z_1$ to the solutions of type $A$, and then use the WKB procedure (called “linear matching” across the turning point) to obtain the dominant WKB solutions beyond $z_1$.

The distant turning point at $z_1$ as indicated in Fig. 3 is given by (using
Eq. (4) for $E$ and ignoring nondominant terms)

$$-\frac{1}{4}z^2h^4 + \frac{1}{2}c^2z^4 \simeq -\frac{1}{2}qh^2,$$

i.e.

$$z_1 \simeq \frac{h^2}{\sqrt{2c^2}} \left(1 - \frac{2qc^2}{h^6}\right) \simeq \frac{h^2}{\sqrt{2c^2}}.$$  

(60)

The WKB solutions have been discussed in the literature.** We obtain in the domain $V > \Re E$ to the left of $z_1$ as the dominant terms of the WKB solutions

$$y_{\text{WKB}}^{(l,z_1)}(z) = \left[-\frac{1}{2}qh^2 + \frac{1}{4}z^2h^4 - \frac{1}{2}c^2z^4\right]^{-1/4} \times \exp \left\{ \int_{z_1}^{z} dz \left[-\frac{1}{2}qh^2 + \frac{1}{4}z^2h^4 - \frac{1}{2}c^2z^4\right]^{1/2} \right\},$$

$$y_{\text{WKB}}^{(r,z_1)}(z) = \left[-\frac{1}{2}qh^2 + \frac{1}{4}z^2h^4 - \frac{1}{2}c^2z^4\right]^{-1/4} \times \exp \left\{ -\int_{z_1}^{z} dz \left[-\frac{1}{2}qh^2 + \frac{1}{4}z^2h^4 - \frac{1}{2}c^2z^4\right]^{1/2} \right\},$$  

(61)

where $z < z_1$, i.e. $z^2h^4/4 > c^2z^4/2$. In using these expressions it has to be remembered that the moduli of the integrals have to be taken.†† To the right of the turning point at $z_1$ these solutions match on to

$$y_{\text{WKB}}^{(r,z_1)}(z) = \left[\frac{1}{2}qh^2 - \frac{1}{4}z^2h^4 + \frac{1}{2}c^2z^4\right]^{-1/4} \times \cos \left\{ \int_{z}^{z_1} dz \left[\frac{1}{2}qh^2 - \frac{1}{4}z^2h^4 + \frac{1}{2}c^2z^4\right]^{1/2} + \frac{\pi}{4} \right\},$$

$$\overline{y}_{\text{WKB}}^{(r,z_1)}(z) = 2\left[\frac{1}{2}qh^2 - \frac{1}{4}z^2h^4 + \frac{1}{2}c^2z^4\right]^{-1/4} \times \sin \left\{ -\int_{z}^{z_1} dz \left[\frac{1}{2}qh^2 - \frac{1}{4}z^2h^4 + \frac{1}{2}c^2z^4\right]^{1/2} + \frac{\pi}{4} \right\}.$$  

(62)

**Ref. [22], p. 291, equations (21), (22) or Ref. [26], Vol. I, Sec.6.2.4.

††Ref. [24], p. 291.
We now come to the algebra of evaluating the integrals in the above solutions. We begin with the exponential factors occurring in Eqs. (61), i.e.

\[ E_\pm = \exp \left\{ \pm \int z^1 \, dz \left[ -\frac{1}{2} q h^2 + \frac{1}{4} z^2 h^4 - \frac{1}{2} c^2 z^4 \right]^{1/2} \right\} \]

\[ = \exp \left\{ \pm \frac{h^6}{8 c^2} \int_z^{z_1} d \left( \frac{2 c^2 z^2}{h^4} \right) \left\{ 1 - \frac{2 c^2 z^2}{h^4} \right\}^{1/2} \left\{ 1 - \frac{2 q}{z^2 h^2} \left[ 1 - \frac{1}{2} c^2 z^4 \right]^{1/2} \right\} \right\} \]

\[ \simeq \exp \left\{ \pm \frac{h^6}{8 c^2} \left\{ \frac{2}{3} \left[ 1 - \frac{2 c^2 z^2}{h^4} \right]^{3/2} \right\}^{z_1} \pm \frac{q h^4}{8 c^2} \int_z^{z_1} \frac{1}{z} d \left( \frac{2 c^2 z^2}{h^4} \right) \right\} \left\{ 1 - \frac{2 q}{z^2 h^2} \left[ 1 - \frac{1}{2} c^2 z^4 \right]^{1/2} \right\} \]

\[ = \exp \left\{ \pm \frac{h^6}{8 c^2} \left\{ \frac{2}{3} \left[ 1 - \frac{2 c^2 z^2}{h^4} \right]^{3/2} \right\} \right\} \left\{ 1 - \frac{2 c^2 z^2}{h^4} \right\}^{1/2} \pm \frac{q}{2} \int_z^{z_1} \frac{d z}{z} \left( \frac{h^4}{2 c^2} - z^2 \right)^{1/2} \left( \frac{h^4}{2 c^2} \right)^{1/2} \right\} \right\} \]

(63)

Here the first part is the exponential factor contained in \( y_A(z), \overline{y}_A(z) \) respectively (cf. Eq. (40)). In the remaining factor we have (looking up Tables of Integrals)

\[ \int_z^{z_1} \frac{d z}{z} \left( \frac{h^4}{2 c^2} - z^2 \right)^{1/2} \]

\[ = \left\{ - \left( \frac{2 c^2}{h^4} \right)^{1/2} \ln \left| \frac{1}{z} \left\{ \left( \frac{h^4}{2 c^2} \right)^{1/2} \right\} \right| \right\}^{z_1} \]

\[ = + \left( \frac{2 c^2}{h^4} \right)^{1/2} \ln \left| \frac{1}{z} \left\{ \left( \frac{h^4}{2 c^2} \right)^{1/2} \right\} \right| \].

Since we are interested in determining the proportionality of two solutions in their common domain of validity we require only the dominant \( z \)-dependence contained in this expression. We obtain this factor by expanding the expression in powers of \( z/z_1 \) (since in the integral \( z < z_1 \)). Thus the above factor yields

\[ \left( \frac{2 c^2}{h^4} \right)^{1/2} \ln \left| \frac{2}{z} \left( \frac{h^4}{2 c^2} \right)^{1/2} \right| \].
so that (cf. Eq. (40))

\[
E_\pm = \exp \left[ \pm \frac{h^6}{8c^2} \left\{ 1 - \frac{2c^2z^2}{h^4} \right\}^{3/2} \mp \frac{q}{2} \ln \left| 2 \left( \frac{h^4}{2c^2} \right)^{1/2} \right| \right] z^{\pm q/2}
\]

\[
= z^{\pm q/2} \left[ 2 \left( \frac{h^4}{2c^2} \right)^{1/2} \right]^{\mp q/2} \exp \left[ \pm i \int^z dz \left\{ - \frac{1}{4} z^2h^4 + \frac{1}{2} c^2 z^4 \right\}^{1/2} \right].
\]

Thus at the left end of the domain of validity of the WKB solutions we have

\[
y^{(l,z_1)}_{\text{WKB}}(z) \simeq \frac{E_+}{\left[ \frac{1}{4} z^2h^4 \right]^{1/4}} \quad \text{and} \quad \overline{y}^{(l,z_1)}_{\text{WKB}}(z) \simeq \frac{E_-}{\left[ \frac{1}{4} z^2h^4 \right]^{1/4}}.
\]

(65)

Comparing these solutions now with the solutions (20a) and (20b), we see that in their common domain of validity

\[
y_A(z) = \beta y^{(l,z_1)}_{\text{WKB}}(z), \quad \overline{y}_A(z) = \overline{\beta} \overline{y}^{(l,z_1)}_{\text{WKB}}(z),
\]

(66)

where

\[
\beta = \left[ \frac{h^2}{2} \right]^{1/2} \left[ 2 \left( \frac{h^2}{2c^2} \right)^{1/2} \right]^{q/2} \quad \text{and} \quad \overline{\beta} = \left[ - \frac{h^2}{2} \right]^{1/2} \left[ 2 \left( \frac{h^2}{2c^2} \right)^{1/2} \right]^{-q/2}
\]

(67a)

or

\[
\frac{\beta}{\overline{\beta}} = \left[ \frac{2h^2}{(2c^2)^{1/2}} \right]^{-q} \frac{(-1)^{q/2}}{\sqrt{-1}}
\]

(67b)

apart from factors \([1+O(1/h^2)]\). In these expressions we have chosen the signs of square roots of \(h^4\) so that the conversion symmetry under replacements \(q \rightarrow -q, h^2 \rightarrow -h^2\) is maintained.

Returning to the even and odd solutions defined by Eqs. (21) we now have

\[
y_{\pm}(z) = \frac{1}{2} [y_A(z) \pm \overline{y}_A(z)]
\]

\[
= \frac{1}{2} \left[ \beta y^{(l,z_1)}_{\text{WKB}}(z) \pm \overline{\beta} \overline{y}^{(l,z_1)}_{\text{WKB}}(z) \right]
\]

\[
= \frac{1}{2} \left[ \beta y^{(r,z_1)}_{\text{WKB}}(z) \pm \overline{\beta} \overline{y}^{(r,z_1)}_{\text{WKB}}(z) \right].
\]

(68)
Now in the domain $z \to \infty$ we have

$$\int_{z_1}^{z} \left[ \frac{1}{2} q h^2 - \frac{1}{4} z^2 h^4 + \frac{1}{2} c^2 z^4 \right]^{1/2} \simeq \int_{z_1}^{z} dz \left[ 1 - \frac{h^4}{4 c^2 z^2} \right]^{1/2} \simeq \left[ \frac{c z^3}{3 \sqrt{2}} \right]_z^{z_1} = \frac{c z^3}{3 \sqrt{2}} - \frac{h^6}{12 c^2}. \quad (69)$$

Inserting this into the solutions (62) and these into (68) we can rewrite the even and odd solutions for $\Re z \to \infty$ as (by separating cosine and sine into their exponential components)

$$y_{\pm}(z) \simeq \frac{1}{2} \left[ \frac{1}{2} c^2 z^4 \right]^{-1/4} \left[ S_+(\pm) \exp \left\{ i \left( \frac{c z^3}{3 \sqrt{2}} - \frac{h^6}{12 c^2} \right) \right\} ight.+ S_-(\pm) \exp \left\{ -i \left( \frac{c z^3}{3 \sqrt{2}} - \frac{h^6}{12 c^2} \right) \right\}], \quad (70)$$

where

$$S_+(\pm) = \left( \frac{1}{2} \beta \pm \frac{1}{i \beta} \right) \exp \left( i \frac{\pi}{4} \right),$$

$$S_-(\pm) = \left( \frac{1}{2} \beta \mp \frac{1}{i \beta} \right) \exp \left( -i \frac{\pi}{4} \right). \quad (71)$$

Imposing the boundary condition that the even and odd solutions have the asymptotic behaviour given by Eq. (59), we see that we have to demand that

$$S_+(\pm) = 0, \quad \text{i.e.} \quad \frac{1}{2} \beta \pm \frac{1}{i \beta} = 0. \quad (72)$$

Inserting expressions (67a) for $\beta$ and $\bar{\beta}$, this equation can be rewritten as

$$(-h^2)^{q/2} = \left( -h^2 \right)^{q/2} \frac{i \beta}{2 \beta} = i \frac{2^{q-1}(-1)^q}{\sqrt{-1}} \left( \frac{h^6}{2 c^2} \right)^{q/2}. \quad (73a)$$

Thus we impose this second boundary condition by making in Eq. (56) the replacement

$$(-h^2)^{q_0/2} \Rightarrow (-)^{q_0-1} \left( \frac{h^6}{2 c^2} \right)^{q_0/2}. \quad (73b)$$
Inserting this into the latter equation we obtain (the factor \( i \) arising from the minus sign on the left of Eq. (73b))

\[
(q - q_0) = \pm i \sqrt{\frac{2}{\pi} \frac{2^{q_0} \left( \frac{\hbar^6}{2c^2} \right)^{q_0/2}}{\left[ \frac{1}{2}(q_0 - 1) \right]!}} e^{-\frac{\hbar^6}{6c^2}}.
\] (74)

with \( q_0 = 1, 3, 5 \ldots \).

### 3.6 The complex eigenvalues

We now return to the expansion of the eigenvalues, i.e. Eq. (33),

\[
E(q, \hbar^2) = \frac{1}{2} q \hbar^2 - \frac{3c^2}{4 \hbar^4} (q^2 + 1) + O\left( \frac{1}{\hbar^{10}} \right).
\]

Expanding about \( q = q_0 \) we obtain

\[
E(q, \hbar^2) = E_0(q_0, \hbar^2) + (q - q_0) \left( \frac{dE}{dq} \right)_{q_0} + \cdots
\]

\[
= E_0(q_0, \hbar^2) + (q - q_0) \frac{\hbar^2}{2} + \cdots. \tag{75}
\]

Clearly the expression for \((q - q_0)\) has to be inserted here giving in the dominant approximation

\[
E = E_0(q_0, \hbar^2) \left( \pm i \right) \frac{2^{q_0} \hbar^2}{(2\pi)^{1/2}} \left[ \frac{1}{2}(q_0 - 1) \right]! \left( \frac{\hbar^6}{2c^2} \right)^{q_0/2} e^{-\frac{\hbar^6}{6c^2}}. \tag{76}
\]

The imaginary part of this expression agrees with the result of Bender and Wu (see formula (3.36) of Ref. [3]) for \( \hbar = 1 \) and in their notation

\[ q_0 = 2K + 1, \quad \frac{\hbar^6}{2c^2} = \epsilon. \]

For comparison with the case of the double well below we note here that the ratio \( \frac{\beta}{\bar{\beta}} \) which we required for the derivation of the result is the ratio of matching coefficients. Hence the result does not involve a specific normalisation of the WKB solutions. This is different in the case of the double well potential that we consider below.
4 The Double-Well Potential

4.1 Defining the problem

In dealing with the case of the symmetric double-well potential, we shall employ basically the same procedure as above. But there are significant differences.

We consider the following equation

\[ \frac{d^2y(z)}{dz^2} + [E - V(z)]y(z) = 0 \]  \hspace{1cm} (77)

with double-well potential

\[ V(z) = v(z) = -\frac{1}{4} z^2 h^4 + \frac{1}{2} c^2 z^4 \]  \hspace{1cm} \text{for } c^2 > 0, \ h^4 > 0. \hspace{1cm} (78)

The minima of \( V(z) \) on either side of the central maximum at \( z = 0 \) are located at

\[ z_\pm = \pm \frac{h^2}{2c} \]  \hspace{1cm} (79)

Fig. 4 The double-well potential.
with
\[ V(z_\pm) = -\frac{h^8}{2^5c^2}, \]
\[ V^{(2)}(z_\pm) = h^4, \quad V^{(3)}(z_\pm) = \pm 6ch^2, \]
\[ V^{(4)}(z_\pm) = 12c^2, \quad V^{(i)}(z_\pm) = 0, \quad i \geq 5. \] (80)

In order to obtain a rough approximation of the eigenvalues we expand the potential about the minima at \( z_\pm \) and obtain
\[
\frac{d^2y}{dz^2} + \left[ E - V(z_\pm) - \frac{1}{2}(z - z_\pm)^2h^4 + O[(z - z_\pm)^3]\right] y = 0. \] (81)

We set
\[
\frac{1}{4}h_\pm^4 \equiv \frac{1}{2}h^4, \quad h_\pm^2 = \sqrt{2}h^2 \quad (82)
\]
(thus we sometimes use \( h^4 \) and sometimes \( h_\pm^4 \)) and
\[
E - V(z_\pm) = \frac{1}{2}q_\pm h_\pm^2 + \frac{\triangle}{h_\pm^4}. \] (83)

With the further substitution
\[
\omega_\pm = h_\pm(z - z_\pm) \] (84)

Eq. (81) becomes
\[
\mathcal{D}_{q_\pm}(\omega_\pm)y(\omega_\pm) = O\left(\frac{1}{h_\pm^4}\right)y, \] (85a)

where
\[
\mathcal{D}_{q_\pm}(\omega_\pm) = 2\frac{d^2}{d\omega^2} + q_\pm - \frac{1}{2}\omega_\pm^2. \] (85b)

By comparison of Eqs. (85a), (85b) with the equation of parabolic cylinder functions \( u(z) \equiv D_\nu(z) \), i.e.
\[
\frac{d^2u(z)}{dz^2} + \left[ \nu + \frac{1}{2} - \frac{1}{4}z^2 \right] u(z) = 0,
\]
we conclude that in the dominant approximation \( q_\pm \) is an odd integer, \( q_0 = 2n + 1, n = 0, 1, 2, \ldots \). Inserting the expression (83) for \( E \) into Eq. (77) we obtain
\[
\frac{d^2y}{dz^2} + \left[ \frac{1}{2}q_\pm h_\pm^2 + \frac{\triangle}{h_\pm^4} - \frac{1}{4}h_\pm^4 U(z) \right] y = 0, \] (86)
where
\[ U(z) = \frac{4}{\hbar_{\pm}} [V(z) - V(z_{\pm})], \] (87a)
and near a minimum at \( z_{\pm} \)
\[ U(z) = (z - z_{\pm})^2 + O[(z - z_{\pm})^3]. \] (87b)

Our basic equation, Eq. (86), is again seen to be invariant under a change of sign of \( z \). Thus again, given one solution, we obtain another by replacing \( z \) by \(-z\).

### 4.2 Three pairs of solutions

We define our first pair of solutions \( y(z) \) as solutions with the proportionality
\[ y(z) \propto \exp \left[ \pm \frac{1}{2} \hbar_{\pm}^2 \int_z^\pm U^{1/2}(z)dz \right]. \] (88)
Evaluating the exponential we can define these as the pair
\[ y_A(z) = A(z) \exp \left[ -\frac{1}{\sqrt{2}} \left\{ \frac{c}{3} z^3 - \frac{h^4}{4c^2} \right\} \right], \]
\[ \bar{y}_A(z) = \bar{A}(z) \exp \left[ +\frac{1}{\sqrt{2}} \left\{ \frac{c}{3} z^3 - \frac{h^4}{4c^2} \right\} \right]. \] (89)

The equation for \( A(z) \) is given by the following equation with upper signs and the equation for \( \bar{A}(z) \) by the following equation with lower signs:
\[ A''(z) = \sqrt{2} \left\{ c z^2 - \frac{h^4}{4c} \right\} A'(z) = \sqrt{2} c z A(z) + \left( \frac{1}{2} q_{\pm} h_{\pm}^2 + \frac{\Delta}{h_{\pm}^4} \right) A(z) = 0. \] (90)

Since
\[ z_{\pm} = \frac{h^2}{2c}, \quad h_{\pm}^2 = \sqrt{2} h^2, \]
and selecting \( z_{\pm} \) with \( q_{\pm} = q \), these equations can be rewritten as
\[ (z_{\pm}^2 - z^2) A'(z) + (q z_{\pm} - z) A(z) = -\frac{\sqrt{2}}{2c} \left[ A''(z) + \frac{\Delta}{h_{\pm}^4} A(z) \right], \] (91a)
\[ (z_{\pm}^2 - z^2) \bar{A}'(z) - (q z_{\pm} + z) \bar{A}(z) = \frac{\sqrt{2}}{2c} \left[ \bar{A}''(z) + \frac{\Delta}{h_{\pm}^4} \bar{A}(z) \right]. \] (91b)
To a first approximation for large $h^2 = 2cz_+$ we can neglect the right hand side. The dominant approximation to $A$ is then the function $A_q$ given by the solution of the first order differential equation

$$D_q A_q(z) = 0, \quad D_q = (z^2 - z^2) \frac{d}{dz} + (qz_+ - z).$$  
(92)

We observe that a change of sign of $z$ in this equation is equivalent to a change of sign of $q$, but the solution is a different one, i.e. $A_q(z) = A_q(-z) = A_{-q}(z)$.

Integration of Eq. (92) yields the following expression

$$A_q(z) = \frac{1}{|z^2 - z^2|^{1/2}} \left| \frac{z - z_+}{z + z_+} \right|^{q/2} = \frac{1}{|z + z_+|^{1/2}(q+1)},$$  
(93)

Looking at Eqs. (91a), (91b) we observe that the solution $\overline{y}_A(q, h^2; z)$ may be obtained from the solution $y_A(q, h^2; z)$ by either changing the sign of $z$ throughout or — alternatively — the signs of both $q$ and $h^2$ (and/or $c$), i.e.

$$\overline{y}_A(q, h^2; z) = y_A(q, h^2; -z) = y_A(-q, -h^2; z).$$  
(94)

Both solutions $y_A(z), \overline{y}_A(z)$ are associated with one and the same expansion for $\triangle$ and hence $E$. We leave the calculation of $\triangle$ to Appendix C. The result is given by Eq. (C.1), i.e.

$$\triangle = -c^2(3q^2 + 1) - \frac{\sqrt{2}c^4}{4h^6} q(17q^2 + 19) + \cdots,$$

$$E(q, h^2) = -\frac{h^8}{2^{\frac{5}{2}}c^2} + \frac{1}{\sqrt{2}}qh^2 - \frac{c^2(3q^2 + 1)}{2h^4} - \frac{\sqrt{2}c^4}{8h^{10}} q(17q^2 + 19) + O\left(\frac{1}{h^{16}}\right).$$  
(95)

The solutions $y_A(z), \overline{y}_A(z)$ derived above are valid in the domains away from the minima,

$$|z - z_\pm| > O\left(\frac{1}{h^2_+}\right).$$

We can define solutions which are even or odd about $z = 0$ as

$$y_\pm(z) = \frac{1}{2}[y_A(q, h^2; z) \pm \overline{y}_A(q, h^2; z)]$$

$$= \frac{1}{2}[y_A(q, h^2; z) \pm y_A(q, h^2; -z)]$$

$$= \frac{1}{2}[y_A(q, h^2; z) \pm y_A(-q, -h^2; z)].$$  
(96)
Considering only the leading approximations of the unnormalised solutions considered explicitly above, we have (since \( A_q(0) = 1/z_+ = A'_q(0) = -q/z_+^2 \))

\[
y_+(q, h^2; 0) = \frac{2c}{h^2}, \quad y_-(q, h^2; 0) = 0, \\
y'_+(q, h^2; 0) = 0, \quad y'_-(q, h^2; 0) = \frac{h^2}{2\sqrt{2}} - \frac{4qc^2}{h^4}.
\]

(97)

Our second pair of solutions, \( y_B(z) \), \( \overline{y}_B(z) \) is obtained around a minimum of the potential. We see already from Eqs. (85a) and (85b), that the solution there is of parabolic cylinder type. This means, in this case we use the Schrödinger equation with the potential \( V(z) \) expanded about \( z_\pm \) as in Eq. (81). Inserting \( \delta^2 \) and setting \( \omega_\pm = h_\pm (z - z_\pm) \), the equation is — with differential operator \( D_q \) as defined by Eq. (85b) —

\[
D_q(\omega_\pm)y(\omega_\pm) = \frac{1}{h^2_\pm} \left[ \pm 2^{5/4} c h^3 \omega_\pm^3 + c^2 \omega_\pm^4 - 2\triangle \right] y(\omega_\pm).
\]

Thus we can write a first solution

\[
y_B(z) = B_q[w_\pm(z)] + O\left(\frac{1}{h^2_\pm}\right), \quad B_q[w_\pm(z)] = \frac{D_{1/4(q-1)}(w_\pm(z))}{\Gamma(1/4(q-1))}, 
\]

and another

\[
\overline{y}_B(z) = y_B(-z) = \overline{B}_q[w_\pm(z)] + O\left(\frac{1}{h^2_\pm}\right)
= B_q[w_\pm(-z)] + O\left(\frac{1}{h^2_\pm}\right).
\]

(98a)

Again the higher order terms along with the eigenvalue expansion in terms of \( q \) are obtained perturbatively.

It is clear that correspondingly we have solutions \( y_C(z) \), \( \overline{y}_C(z) \) with complex variables and \( C_q(w) \) given by Eq. (23) with appropriate change of parameters to those of the present case. Thus

\[
y_C(z) = C_q[w_\pm(-z)] + O\left(\frac{1}{h^2_\pm}\right), \\
C_q[w_\pm(-z)] = \frac{D_{-1/4(q+1)}(iw_\pm(-z))2^{1/4(q+1)}}{[-1/4(q+1)]!},
\]

(99a)
\[ \overline{y}_C(z) = y_C(-z) = \overline{C}_q[w_\pm(-z)] = C_q[w_\pm(+z)] + O \left( \frac{1}{h_\pm^2} \right). \] (99b)

These are solutions again around a minimum and with \( y_B(z), \overline{y}_C(z) \) providing a pair of decreasing asymptotic solutions there (or correspondingly \( \overline{y}_B(z), y_C(z) \)). We draw attention to two additional points. Since \( w_\pm(-z) = -h_\pm(z + z_\pm) \), we have \( w_\pm(-z_\pm) = -2h_\pm z_\pm \), but \( w_\pm(z_\pm) = 0 \). Moreover, in view of the factor “\( i \)” in the argument of \( C_q \) the solutions \( y_A, y_C \) have the same exponential behaviour near a minimum.

### 4.3 Matching of solutions

Next we consider the proportionality of solutions \( y_A(z) \) and \( y_B(z) \). Evaluating the exponential factor contained in \( y_A(z) \) of Eq. (89) for \( z \to z_\pm \), we have (cf. (87b))

\[
\exp \left[ -\frac{1}{2} h_\pm^2 \int z U^{1/2}(z) \, dz \right] \approx \exp \left[ -\frac{1}{2} h_\pm^2 \int (z - z_\pm) \, dz \right] = \exp \left[ -\frac{1}{2} h_\pm^2 \left( \frac{1}{2} z^2 - z z_\pm \right) \right] = \exp \left[ -\frac{1}{4} h_\pm^2 (z - z_\pm)^2 \right] \exp \left[ \frac{1}{4} h_\pm^2 z_\pm^2 \right].
\]

Allowing \( z \) to approach \( z_\pm \) in the solution \( y_A(z) \), we have

\[
y_A(z) \approx \frac{z - z_\pm}{2 z_\pm} \frac{1}{[2 z_\pm]^{1/2}(q+1)} e^{\frac{1}{2} h_\pm^2 z_\pm^2} e^{-\frac{1}{4} h_\pm^2 (z - z_\pm)^2} = \frac{(w_\pm(z_\pm))^{1/2}(q-1)}{(2 z_\pm)^{1/2}(q+1)} e^{\frac{1}{2} h_\pm^2 z_\pm^2} e^{-\frac{1}{4} w_\pm^2}. \quad (100)
\]

Recalling that around \( \arg w_\pm \sim 0 \), the dominant term in the power expansion of the parabolic cylinder function for large values of its argument is given by

\[ D_\nu(w_\pm) \simeq w_\pm^\nu e^{-w_\pm^2/4}, \]

and comparing with Eq. (98a) we see that (considering only dominant contributions) in their common domain of validity

\[
y_A(z) = \frac{1}{\alpha} y_B(z), \quad \alpha = \frac{(h_\pm)^{1/2}(q-1)(2 z_\pm)^{1/2}(q+1)}{2^{1/2}(q-1)[\frac{1}{4}(q-1)]} e^{-\frac{1}{4} h_\pm^2 z_\pm^2} \left[ 1 + O \left( \frac{1}{h_\pm^2} \right) \right]. \quad (101)
\]
Similarly we obtain in approaching $z_+$:
\[
\overline{y}_A(z) \simeq \frac{(2z_+)^{\frac{1}{2}(q-1)}}{(z - z_+)^{\frac{1}{2}(q+1)}} e^{-\frac{1}{2}h_+^2 z_+^2} e^{\frac{1}{4}h_+^2(z-z_+)^2} \tag{102}
\]

and
\[
\overline{y}_C(z) \simeq \frac{D_{-\frac{1}{2}(q+1)}(i w_+(z)) 2^{\frac{1}{2}(q+1)}}{[-\frac{1}{4}(q + 1)]!} \frac{2^{\frac{1}{2}(q+1)} e^{\frac{1}{4}h_+^2(z-z_+)^2}}{[-\frac{1}{4}(q + 1)]! [ih_+(z - z_+)]^{\frac{1}{2}(q+1)}}. \tag{103}
\]

Therefore in their common domain of validity
\[
\overline{y}_A(z) = \frac{1}{\alpha} \overline{y}_C(z), \quad \alpha = \frac{2^{\frac{1}{2}(q+1)} e^{\frac{1}{4}h_+^2 z_+^2}}{(2z_+)^{\frac{1}{2}(q-1)}(-h_+^2)^{\frac{1}{2}(q+1)}[-\frac{1}{4}(q + 1)]!} \left[1 + O\left(\frac{1}{h_+^2}\right)\right]. \tag{104}
\]

We have thus found three pairs of solutions: The two solutions of type $A$ are valid in regions away from the minima, and are both in their parameter-dependence asymptotically decreasing there and permit us therefore to define the extensions of the solutions $y_\pm$ which are respectively even and odd about $z = 0$ to the minima. The pair of solutions of type $B$ is defined around $\arg z = 0, \pi$ and the solutions of type $C$ around $\arg z = \pm \pi/2$. The next aspect to be considered is that of boundary conditions. We have to impose boundary conditions at the minima and at the origin. The solutions in terms of parabolic cylinder functions have a wide range of validity, even above the turning points, but it is clear that none of the above solutions can be used at the top of the central barrier. Thus it is unavoidable to appeal to (other and that means) WKB methods to apply the necessary boundary conditions at that point. The involvement of these WKB solutions leads to problems since, basically, they assume large quantum numbers. Various investigations, such as those of Refs. [17], [18], [19], [21], therefore struggle to overcome this to a good approximation. We achieve the same goal (i.e. approximation) as such corrections here by demanding our basic perturbation solutions to be interconvertible on the basis of the parameter symmetries of the original equation.

4.4 Boundary conditions at the minima

(A) Formulation of the boundary conditions
The present case of the double-well potential differs from that of the simple harmonic oscillator potential in having two minima instead of one.

![Diagram of double-well potential]

Fig. 5 Behaviour of fundamental wave functions.

Since it is more probable to find a particle in the region of a minimum than elsewhere, we naturally expect the wave function there to be similar to that of the harmonic oscillator, and this means at both minima. Thus the most basic solution would be even with maxima at $z_{\pm}$, as indicated in Fig. 5. However, an even wave function can also pass through zero at these points, as indicated in Fig. 5. The odd wave function then exhibits a correspondingly opposite behaviour, as indicated there. At $\Re z \to \pm \infty$ we require the wave functions to vanish so that they are square integrable. We have therefore the following two sets of boundary conditions at the local minima of the double well potential:

$$
y'_+(z_{\pm}) = 0, \quad y_+(z_{\pm}) \neq 0,
$$
$$
y_-(z_{\pm}) = 0, \quad y'_-(z_{\pm}) \neq 0
$$

(105)

and

$$
y_+(z_{\pm}) = 0, \quad y'_+(z_{\pm}) \neq 0,
$$
$$
y'_-(z_{\pm}) = 0, \quad y_-(z_{\pm}) \neq 0.
$$

(106)
We have
\[ y_\pm(z_\pm) = \frac{1}{2}[y_A(z) ± y_A(z)]_{z \to z_\pm} = \frac{1}{2} \left[ \frac{1}{\alpha} y_B(z_\pm) ± \frac{1}{\alpha} y_C(z_\pm) \right] \] (107)

and
\[ y'_\pm(z_\pm) = \frac{1}{2} \left[ \frac{1}{\alpha} y'_B(z_\pm) ± \frac{1}{\alpha} y'_C(z_\pm) \right]. \] (108)

Hence the conditions (105), (106) imply
\[ \frac{y_B(z_\pm)}{y_C(z_\pm)} = \mp \frac{\alpha}{\alpha}, \quad \text{and} \quad \frac{y'_B(z_\pm)}{y'_C(z_\pm)} = \mp \frac{\alpha}{\alpha}. \] (109)

**(B) Evaluation of the boundary conditions**

Inserting into the first of Eqs. (109) the dominant approximations we obtain (cf. also Eqs. (B.1a) and (B.1b))
\[ 1 = \mp \frac{\alpha}{\alpha} = \mp (-1)^{\frac{1}{2}(q+1)} \left( \frac{h_0^2}{2} \right)^{q/2}(2z_+)^q \left[ \frac{1}{4}(q+1)! \right] \left[ \frac{1}{4}(q-1)! \right] \sin \left( \frac{\pi}{4}(q+1) \right) e^{-\frac{1}{2}h_0^2 z_+^2} \]
\[ = \mp (-1)^{\frac{1}{2}(q+1)} \frac{\pi (h_0^2)^{q/2}(2z_+)^q}{2^{q/2}[\frac{1}{4}(q-1)!][\frac{1}{4}(q-3)!]} \sin \left( \frac{\pi}{4}(q+1) \right) \]
\[ = \mp (-1)^{\frac{1}{2}(q+1)} \frac{\pi (h_0^2)^{q/2}(2z_+)^q}{2^{q/2}[\frac{1}{4}(q-1)!][\frac{1}{4}(q-3)!]} \sin \left( \frac{\pi}{4}(q+1) \right) e^{-\frac{1}{2}h_0^2 z_+^2}, \] (110)

where we used first the reflection formula and then the duplication formula. Thus
\[ \sin \left( \frac{\pi}{4}(q+1) \right) = \mp (-1)^{\frac{1}{2}(q+1)} \sqrt{\frac{2}{\pi} (h_0^2)^{q/2}(2z_+)^q} e^{-\frac{1}{2}h_0^2 z_+^2}, \] (111)

Using formulae derived in Appendix B we can rewrite the second of Eqs. (109) as
\[ \frac{y'_B(z_\pm)}{y'_C(z_\pm)} = -i \cot \left( \frac{\pi}{4}(q+1) \right) \equiv -i \cot \left( \frac{\pi}{4}(q+1) \right) = \mp \frac{\alpha}{\alpha}. \] (112)
Using Eq. (110) this equation can be written

$$-i \cos \left\{ \frac{\pi}{4} (q + 1) \right\} = \mp (-1)^{\frac{q}{4}(q+1)} \sqrt{\frac{\pi (h_{+}^{2})^{q/2}}{2 \left[ \frac{1}{2} (q - 1) \right]!}} \frac{2^{q}}{2 \pi} \left( h_{+}^{2} \right)^{q/2} (2z_{+})^{q} e^{-\frac{1}{2} h_{+}^{2} z_{+}^{2}}. \quad (113)$$

Now

$$\sin \left\{ \frac{\pi}{4} (q + 1) \right\} \simeq \sin \left\{ \frac{\pi}{4} (q_{0} + 1) \right\} + \frac{\pi}{4} (q - q_{0}) \cos \left\{ \frac{\pi}{4} (q_{0} + 1) \right\} + \cdots$$

$$\simeq (-1)^{\frac{1}{4}(q_{0}+1)} (q - q_{0}) \frac{\pi}{4} \quad \text{for} \quad q_{0} = 3, 7, 11, \ldots. \quad (114)$$

and

$$\cos \left\{ \frac{\pi}{4} (q + 1) \right\} \simeq \cos \left\{ \frac{\pi}{4} (q_{0} + 1) \right\} - \frac{\pi}{4} (q - q_{0}) \sin \left\{ \frac{\pi}{4} (q_{0} + 1) \right\} + \cdots$$

$$\simeq -(-1)^{\frac{1}{4}(q_{0}+1)} (q - q_{0}) \frac{\pi}{4} \quad \text{for} \quad q_{0} = 1, 5, 9, \ldots$$

$$= -(q - q_{0}) \frac{\pi}{4} (-1)^{\frac{1}{4}(q_{0}+1)} (-1)^{1/2}. \quad (115)$$

Thus altogether we obtain from the boundary conditions at $z_{+}$ (and correspondingly from those at $z_{-}$)

$$(q - q_{0}) \simeq \mp 4 \sqrt{\frac{1}{2 \pi} \left( h_{+}^{2} \right)^{q_{0}/2}(2z_{+})^{q_{0}}} e^{-\frac{1}{2} h_{+}^{2} z_{+}^{2}}, \quad q_{0} = 1, 3, 5, \ldots. \quad (116)$$

In Appendix E (after calculation of turning points) we rederive this relation using the WKB solutions from above the turning points matched (linearly) to their counterparts below the turning points and then evaluated at the minimum.

In summary: We needed the solutions of type A for the definition of even and odd solutions. Since the type A solutions are not valid at the minima, we matched them to the solutions of types B and C which are valid there and hence permit the imposition of boundary conditions at the minima.

4.5 Boundary conditions at the origin
(A) Formulation of the boundary conditions
Since our even and odd solutions are defined to be even or odd with respect to the origin, we must also demand this behaviour here along with a nonvanishing Wronskian.

Fig. 6 Turning points $z_0, z_1$.

Hence we have to impose at $z = 0$ the conditions

\[
\begin{align*}
  y_-(0) &= 0, \quad y'_-(0) \neq 0, \\
  y_+(0) &\neq 0, \quad y'_+(0) = 0.
\end{align*}
\]  
\tag{117}

Thus we require the extension of our solutions to the region around the local maximum at $z = 0$. We do this with the help of WKB solutions. We deduce from Eq. (97) that the two turning points at $z_0$ and $z_1$ to the right of the origin are given by

\[
\frac{1}{2} q h_+^2 + \frac{\Delta}{h_+^4} - \frac{1}{4} h_+^4 U(z) = 0,
\]  
\tag{118}

i.e.

\[
\frac{1}{2} q h_+^2 + \frac{1}{4} z^2 h_+^4 - \frac{1}{2} c^2 z^4 - \frac{h_+^8}{2 c^2} = O\left(\frac{\Delta}{h_+^4}\right).
\]
Using $z_+=h^2/2c$, one finds that

$$z_0 = \left\{ \frac{h^4}{4c^2} - \sqrt{\frac{qh^2}{c^2}} + O\left(\frac{\Delta h_+}{h^4}\right) \right\}^{1/2} = \frac{h^2}{2c} - \frac{(2q^2)^{1/4}}{h} + \frac{2^{1/2}cq}{h^4} + O\left(\frac{1}{h^5}\right)$$

and

$$z_1 = \left\{ \frac{h^4}{4c^2} + \sqrt{\frac{qh^2}{c^2}} + O\left(\frac{\Delta h_+}{h^4}\right) \right\}^{1/2} \approx \frac{h^2}{2c} + \frac{(2q^2)^{1/4}}{h}. \quad (120)$$

The height of the potential at these points is

$$V(z)|_{z_0, z_1} \simeq -\frac{h^8}{2^5c^2} + \frac{qh}{2^{1/2}}.$$ 

Thus for large values of $h^2$ the turning points are very close to minima of the potential for nonasymptotically large values of $q$.

(B) Evaluation of the boundary conditions

We now proceed to evaluate the boundary conditions (117). In the domain $0 < z < z_0$, i.e. to the left of $z_0$ where $V > E$, the dominant terms of the WKB solutions are*

$$y^{(l, z_0)}_{WKB}(z) = \left[ -\frac{1}{2}qh^2_+ + \frac{1}{4}h_+^4U(z) \right]^{-1/4} \times \exp\left( -\int_z^{z_0} dz \left[ -\frac{1}{2}qh^2_+ + \frac{1}{4}h_+^4U(z) \right]^{1/2} \right) \quad (121)$$

and

$$\overline{y}^{(l, z_0)}_{WKB}(z) = \left[ -\frac{1}{2}qh^2_+ + \frac{1}{4}h_+^4U(z) \right]^{-1/4} \times \exp\left( \int_z^{z_0} dz \left[ -\frac{1}{2}qh^2_+ + \frac{1}{4}h_+^4U(z) \right]^{1/2} \right). \quad (122)$$

In order to be able to extend the even and odd solutions to $z = 0$, we have to match $y_A(z), \overline{y}_A(z)$ to $y^{(l, z_0)}_{WKB}(z)$ and $\overline{y}^{(l, z_0)}_{WKB}(z)$. We therefore have to consider

*The superscript $(l, z_0)$ means “to the left of $z_0$.”
the exponential factors occurring in (121) and (122) and consider both types of solutions in a domain approaching but not reaching the minimum of the potential at \( z_+ \). Thus we consider in the domain \(|z - z_+| > (2q/h^2_+)^{1/2}\):

\[
I_1 = \int_{z_0}^{z_0} dz \left[ -\frac{1}{2}qh^2_+ + \frac{1}{4}h^4_+ U(z) \right]^{1/2} \\
\simeq \pm \frac{1}{2}h^2_+ \int_{z_0}^{z_0} dz \left[ (z - z_+)^2 - \frac{2q}{h^2_+} \right]^{1/2} \\
= \pm \frac{1}{2}h^2_+ \int_{z=z_+}^{z_0-z_+} dz' \left( z'^2 - \frac{2q}{h^2_+} \right)^{1/2} \\
= \pm \frac{1}{2}h^2_+ \left[ \frac{1}{2}z' \left( z'^2 - \frac{2q}{h^2_+} \right)^{1/2} \right]^{z_0-z_+}_{z=z_+} \\
- \frac{q}{h^2_+} \ln \left| z' + \left( z'^2 - \frac{2q}{h^2_+} \right)^{1/2} \right|^{z_0-z_+}_{z-z_+}. \quad (123)
\]

Evaluating this we have (with \( z_0 - z_+ = -(2q^2)^{1/4}/h = -(2q/h^2_+)^{1/2} \))

\[
\pm I_1 \simeq \frac{1}{2}h^2_+ \left\{ \frac{1}{2}z'^2 \left( 1 - \frac{q}{h^2_+}z'^2 \right) \right\} \quad z' = -(2q/h^2_+)^{1/2} \\
- \frac{q}{h^2_+} \ln \left| - \left( \frac{2q}{h^2_+} \right)^{1/2} + O \left( \frac{1}{h^5} \right) \right| - \frac{1}{2} \left( z - z_+ \right) \left\{ \left( z - z_+ \right)^2 - \frac{2q}{h^2_+} \right\}^{1/2} \\
+ \frac{q}{h^2_+} \ln \left| (z - z_+) + \left\{ \left( z - z_+ \right)^2 - \frac{2q}{h^2_+} \right\}^{1/2} \right| \\
\simeq \frac{1}{4}q + \frac{1}{4}q \ln \left| \frac{h^2_+}{2q} \right| - \frac{1}{4}h^2_+ (z - z_+)^2 + \frac{1}{2}q \ln |2(z - z_+)|. \quad (124)
\]

In identifying the WKB exponentials we recall that \( y_{\text{WKB}} \) is exponentially increasing and \( y_{\text{WKB}} \) exponentially decreasing. Hence we have for \( y_{\text{WKB}} \) the exponential factor

\[
\exp \left( -\int_{z_0}^{z} dz \left[ -\frac{1}{2}qh^2_+ + \frac{1}{4}h^4_+ U(z) \right]^{1/2} \right) \\
\simeq |z - z_+|^{q/2} e^{\frac{1}{4}q} \left( \frac{h^2_+}{2q} \right)^{q/4} \left( \frac{q}{4} \right)^{-q/4} e^{-\frac{1}{4}(z-z_+)^2 h^2_+}. \quad (125a)
\]
We observe here that the WKB solution involves unavoidably the quantum-number-dependent factors \( \exp(q/4) \) and \( (q/4)^{q/4} \) which do not appear as such in the perturbation solutions. The only way to relate these solutions is with the help of the Stirling formula which converts the product or ratio of such factors into factorials such as those inserted from the beginning into the unperturbed solutions (98a) and (99a). However, Stirling’s formula is the dominant term of the asymptotic expansion of a factorial or gamma function and thus assumes the argument \( \propto q \sim 2n+1 \) to be large (it is known, of course, that the Stirling approximation is amazingly good even for small values of the argument). Thus, using the Stirling formula

\[
\frac{z!}{\sqrt{2\pi z^{3/2}}} \approx e^{-z} \frac{z^{1/2}}{\sqrt{2\pi}},
\]

we can rewrite the exponential as

\[
\exp \left( -\int_{z_0}^{z} \left[ -\frac{1}{2} q h_+^2 + \frac{1}{4} h_+^4 U(z) \right]^{1/2} \right) \\
\approx (2\pi)^{1/2} \left| \frac{z-z_+}{\frac{1}{4}(q-1)!} \right|^{q/4} \left( \frac{1}{2} h_+^2 \right)^{q/4} e^{-\frac{1}{4}(z-z_+)^2 h_+^2}.
\]

Here \( q/4 \) was assumed to be large but we write \( \left[ \frac{1}{4}(q-1)! \right] \) since this is the factor appearing in the solution (98a). We see therefore, since there is no way to obtain an exact leading order approximation with Stirling’s formula for small values of \( q \), the results necessarily require adjustment or normalisation there in the \( q \)-dependence. This is the aspect investigated by Furry [21].

Since correspondingly

\[
\left[ -\frac{1}{2} q h_+^2 + \frac{1}{4} h_+^4 U(z) \right]^{1/2} \approx \frac{2^{1/2}}{(z-z_+)^{1/2}(h_+^4)^{1/4}},
\]

we obtain

\[
y_{\text{WKB}}^{(l,z_0)}(z) \approx \frac{2\sqrt{\pi}}{(h_+^4)^{1/4} \left| \frac{1}{4}(q-1)! \right|^{q/4} \left( \frac{1}{2} h_+^2 \right)^{q/4} e^{-\frac{1}{4}(z-z_+)^2 h_+^2}} \left( \frac{2q}{h_+^2} \right)^{1/2}.
\]

This expression is valid to the left of the turning point at \( z_0 \) above the minimum at \( z_+ \).

In a corresponding manner — i.e. using Stirling’s formula (and not the inversion relation) — we have

\[
y_{\text{WKB}}^{(l,z_0)}(z) = \frac{1}{\sqrt{\pi}(h_+^4)^{1/4} \left| z-z_+ \right|^{\frac{1}{4}(q+1)}} \left( \frac{1}{2} h_+^2 \right)^{-q/4} e^{\frac{1}{4}(z-z_+)^2 h_+^2},
\]

(127)
where \([\frac{1}{4}(q-3)]!\) was written as \([\frac{1}{4}(q-3)]!\) for \(q\) large. Comparing for \(z \to z_+\) the WKB solutions (126), (127) with the type-A solutions (100), (104) we obtain in leading order (i.e. multiplied by \((1+O(1/h^2))\)) the proportionality constants \(\gamma, \overline{\gamma}\) of the matching relations

\[
y^{(l,z_0)}_{WKB}(z) = \gamma y_A(z), \quad \overline{y^{(l,z_0)}_{WKB}}(z) = \overline{\gamma} \overline{y_A}(z),
\]

i.e.

\[
\gamma = \frac{2\sqrt{\pi}}{(h_+^4)^{1/4}[\frac{1}{4}(q-1)]!} \left(\frac{1}{2}h_+^2\right)^{q/4} (2z_+)^{1/2(q+1)} e^{-\frac{1}{2}h_+^2 z_+^2},
\]

(129a)

and

\[
\overline{\gamma} = \frac{[\frac{1}{4}(q-3)]!}{\sqrt{\pi}(h_+^4)^{1/4}} \left(\frac{1}{2}h_+^2\right)^{-q/4} (2z_+)^{-1/2(q-1)} e^{\frac{1}{2}h_+^2 z_+^2}.
\]

(129b)

Using again the duplication formula\(^1\) the ratio of these constants becomes

\[
\frac{\gamma}{\overline{\gamma}} = \sqrt{\frac{2\pi}{\left[\frac{1}{4}(q-1)\right]!}} \frac{(h_+^2)^{q/2}(2z_+)^q}{e^{-\frac{1}{2}h_+^2 z_+^2}}.
\]

(130)

Since the factorials \([\frac{1}{4}(q-1)]!, [\frac{1}{4}(q-3)]!\) are really correct replacements of \([\frac{1}{4}(q)]!\) only for \(q\) large, this result is somewhat imprecise. However, it is our philosophy here that the factorials with factors occurring in the perturbation solutions are the more natural and hence correct expressions, as the results also seem to support. The relation (130) is used in Appendix E for the calculation of the tunneling deviation \(q - q_0\) by using the usual (i.e. linearly matched) WKB solutions, and is shown to reproduce correctly the result (116) which was obtained with our perturbation solutions from the boundary conditions at a minimum.

Returning to the even and odd solutions (96) we have

\[
y_{\pm}(z) = \frac{1}{2} [y_A(z) \pm \overline{y_A}(z)] = \frac{1}{2\gamma} y^{(l,z_0)}_{WKB}(z) \pm \frac{1}{2\overline{\gamma}} \overline{y^{(l,z_0)}_{WKB}}(z).
\]

(131)

Applying the boundary conditions (117) we obtain

\[
\frac{y^{(l,z_0)}_{WKB}(0)}{\overline{y^{(l,z_0)}_{WKB}}(0)} = \frac{\gamma}{\overline{\gamma}}, \quad \frac{y^{(l,z_0)\prime}_{WKB}(0)}{\overline{y^{(l,z_0)\prime}_{WKB}}(0)} = -\frac{\gamma}{\overline{\gamma}}.
\]

(132)

\(^1\)In the present case as

\[
[\frac{1}{4}(q-1)]![\frac{1}{4}(q-3)]! = \sqrt{\pi} 2^{-\frac{1}{2}(q-1)} \left[\frac{1}{2}(q-1)\right]!.
\]
Thus we have to consider the behaviour of the integrals occurring in the solutions (121), (122) near $z = 0$. We have

\[
I_2(z) \equiv \int_z^{z_0} dz \left[ -\frac{1}{2} q h_+^2 + \frac{1}{4} h_+^4 U(z) \right]^{1/2}
\]

\[
= \int_z^{z_0} dz \left[ -\frac{1}{2} q h_+^2 - \frac{1}{4} z^2 h^4 + \frac{1}{2} c^2 z^4 + \frac{h^8}{2^5 c^2} \right]^{1/2}
\]

\[
= \int_z^{z_0} dz \left[ \frac{1}{2} \left( \frac{h_+^4}{2^2 c} - c z^2 \right)^2 - \frac{1}{2} q h_+^2 \right]^{1/2}
\]

\[
= \frac{c}{\sqrt{2}} \int_z^{z_0} dz \left[ \left( \frac{h_+^4}{4 c^2} - \sqrt{q h_+} - z^2 \right) \left( \frac{h_+^4}{4 c^2} + \sqrt{q h_+} - z^2 \right) \right]^{1/2}.
\]

Setting

\[
b^2 = \frac{h_+^4}{4 c^2} - \sqrt{q h_+} \simeq z_0^2, \quad a^2 = \frac{h_+^4}{4 c^2} + \sqrt{q h_+}, \quad b^2 < a^2, \quad (133)
\]

we can rewrite the integral as

\[
I_2(z) = \frac{c}{\sqrt{2}} \int_z^{b} dz \sqrt{(a^2 - z^2)(b^2 - z^2)}. \]

The integral appearing here is an elliptic integral which can be looked up in Ref. [29]. The elliptic modulus $k$ (with $k'^2 = 1 - k^2$) and an expression $u$ appearing in the integral are defined by

\[
k^2 = \frac{b^2}{a^2} = 1 - u, \quad u = \frac{8 c}{h_+^3} \sqrt{q} \equiv G \sqrt{2q}, \quad G^2 = \frac{8 \sqrt{2 c^2}}{h_+^6}, \quad (134a)
\]

so that

\[
a = \frac{h_+^2}{2c} [1 + u]^{1/2}. \quad (134b)
\]

The integral $I_2(z)$ evaluated at $z = 0$ is then given in Ref. [29] by

\[
I_2(0) = \frac{c a^3}{3 \sqrt{2}} [(1 + k^2) E(k) - k^2 K(k)]
\]

\[
= \frac{h_+^6}{12 \sqrt{2 c^2}} \sqrt{1 + u} [E(k) - u K(k)],
\]

\[
= \frac{2}{3 G^2} \sqrt{1 + u} [E(k) - u K(k)], \quad (135a)
\]

‡See Ref. [29], formulae 220.05, p. 60 and 361.19, p. 213.
where $K(k)$ and $E(k)$ are the complete elliptic integrals of the first and second kinds respectively. Here we are interested in the behaviour of the integral in the domain of large $h^6/c^2$ which implies small $G^2$. The nontrivial expansions are derived in Appendix F, where the result is shown to be (with $q \approx q_0 = 2n + 1, n = 0, 1, 2, \ldots$)

$$I_2(0) = \pm \frac{q}{4} \pm \frac{1}{2} \frac{h^6}{12c^2} \mp \frac{q}{2} \ln \left| \frac{2h^3}{2^{1/4} c q^{1/2}} \right|$$

$$= \pm \frac{2}{3G^2} \pm \left(n + \frac{1}{2}\right) \ln \left(\frac{G}{4}\right) \pm \frac{1}{2} \left(n + \frac{1}{2}\right) \ln \left(n + \frac{1}{2}\right)$$

$$\mp \frac{1}{2} \left(n + \frac{1}{2}\right).$$

(135b)

in agreement with Ref. [10]. Since the integral is to be positive (as required in the WKB solutions) we have to take the upper signs. It then follows that (again in each case in leading order)

$$y^{(l,z_0)}_{WKB}(z)|_{z=0} \approx \frac{(\frac{2h^6}{c^2})^{q/4}}{2^{3q/8} (\frac{h^6}{2^{3/4} c^2})^{1/4} (\frac{q}{4})^{q/4} e^{-q/4} e^{-h^6/12\sqrt{2}c^2}} ,$$

(136)

where $h^8/2^5 c^2 = -V(z_{\pm})$. Using Stirling’s formula we can write this

$$y^{(l,z_0)}_{WKB}(z)|_{z=0} \approx \frac{\sqrt{2\pi} \left(\frac{2h^8}{c^2} - \frac{1}{2} h^8 \right)^{1/4} \left(\frac{q}{4}\right)^{q/4} e^{-q/4} e^{-h^6/12\sqrt{2}c^2}}{\left(\frac{h^8}{2^{3/4} c^2}\right)^{1/4} \left[\frac{1}{4}(q - 1)\right]!} .$$

(137)

Correspondingly we find

$$\overline{y}^{(l,z_0)}_{WKB}(z)|_{z=0} \approx \sqrt{\frac{1}{2\pi}} \frac{[\frac{1}{4}(q - 3)]!}{\left(\frac{2h^8}{c^2} - \frac{1}{2} h^8 \right)^{1/4} \left(\frac{q}{4}\right)^{q/4} e^{-q/4} e^{-h^6/12\sqrt{2}c^2}}$$

(138)

and

$$\frac{d}{dz} y^{(l,z_0)}_{WKB}(z)|_{z=0} \approx \left(\frac{h^8}{2^5 c^2}\right)^{1/4} \left(2\pi\right)^{1/2} \left(\frac{2h^8}{c^2} - \frac{1}{2} h^8 \right)^{1/4} \left[\frac{1}{4}(q - 1)\right]! e^{-h^6/12\sqrt{2}c^2}$$

(139)

and

$$\frac{d}{dz} \overline{y}^{(l,z_0)}_{WKB}(z)|_{z=0} \approx -\left(\frac{h^8}{2^5 c^2}\right)^{1/4} \frac{[\frac{1}{4}(q - 3)]!}{\left(2\pi\right)^{1/2} \left(\frac{2h^8}{c^2} - \frac{1}{2} h^8 \right)^{1/4} \left[\frac{1}{4}(q - 1)\right]!} e^{-h^6/12\sqrt{2}c^2} .$$

(140)

The expansion of $I_2$ used in Ref. [10] misses an $n$-dependent power of 2 in the result.
With these expressions we obtain now from Eqs. (132) — on using once again the duplication formula in the same form as above —

\[
\sqrt{2\pi} \frac{2^{q/2}}{[\frac{1}{2}(q-1)!]} \left( \frac{2h^6}{c^2} \frac{1}{2^{3/2}} \right)^{q/2} e^{-\frac{h^6}{6\sqrt{2}c^2}} = \frac{\gamma}{\gamma}.
\] (141)

Comparing this result with that of Eq. (130), we can therefore impose the boundary conditions at \( z = 0 \) by making in Eq. (116) the replacement

\[
(h_+^2)^{q/2}(2z_+)^q e^{-\frac{h_+^2z_+^2}{6}} \Rightarrow 2^q \left( \frac{h^6}{2^{3/2}c^2} \right)^{q/2} e^{-\frac{h_0^6}{6\sqrt{2}c^2}}.
\] (142)

A corresponding relation holds for \( h_- \) and \( z_- \) replaced by \( h_+ \) and \( z_+ \). Inserting the expressions for \( h_+ \) and \( z_+ \) in terms of \( h \), we see that the relation is really an identity (the pre-exponential factors on the left and on the right being equal) with the exponential on the left being an approximation of the exponential on the right (which contains the full action of the instanton). This is our second condition in the present case of the double well potential.

### 4.6 Eigenvalues and level splitting

We now insert the relation (142) into Eq. (116) with \( q_0 = 2n + 1, n = 0, 1, 2, \ldots \), and obtain

\[
(q - q_0) \simeq 4\sqrt{\frac{1}{2\pi} \frac{2^{q_0}(\frac{h^6}{2})^{q_0/2}}{2^{q_0/4} \left[ \frac{1}{2}(q_0 - 1)! \right]!}} e^{-\frac{h^6}{6\sqrt{2}c^2}}, \quad q_0 = 1, 3, 5, \ldots.
\] (143)

We obtain the energy \( E(q, h^2) \) and hence the splitting of asymptotically degenerate energy levels with the help of Eq. (116). Expanding this around an odd integer \( q_0 \) we have

\[
E(q, h^2) \simeq E_0(q_0, h^2) + (q - q_0) \left( \frac{\partial E}{\partial q} \right)_{q_0}
\]

\[
\simeq E_0(q_0, h^2) + (q - q_0) \frac{h^2}{\sqrt{2}}.
\] (144)

Inserting here the result (143) we obtain for \( E(q_0, h^2) \) the split expressions

\[
E_{\pm}(q_0, h^2) \simeq E_0(q_0, h^2) \pm \frac{2^{q_0+1}h^2(\frac{h^6}{2c^2})^{q_0/2}}{\sqrt{\pi}2^{q_0/4} \left[ \frac{1}{2}(q_0 - 1)! \right]!} e^{-\frac{h_0^6}{6\sqrt{2}c^2}}, \quad q_0 = 1, 3, 5, \ldots.
\] (145)
where \( E_0(q_0, h^2) \) is given by Eq. (C.1), i.e. 
\[
E_0(q_0, h^2) = -\frac{h^8}{2^5 c^2} + \frac{1}{\sqrt{2}} q_0 h^2 - \frac{c^2(3q^2 + 1)}{2h^4} + O\left(\frac{1}{h^{10}}\right).
\]

Thus
\[
\Delta E(q_0, h^2) = E_-(q_0, h^2) - E_+(q_0, h^2)
\]
\[
\approx \frac{2^{n^2} h^2}{\sqrt{\pi} 2^{q_0/4}[1/2 (q_0 - 1)]} \left(\frac{h^6}{2c^2}\right)^{q_0/2} e^{-\frac{h^6}{2^{1/2} a c^2}} , \quad \text{(mass } m_0 = \frac{1}{2})
\]
\[
= 2^{(2n+9)/4} \frac{h^2}{\sqrt{\pi} n!} \left(\frac{h^6}{c^2}\right)^{n+1/2} e^{-\frac{h^6}{2^{1/2} a c^2}} . \quad (146)
\]

Combining Eqs. (144) and (E.14) with (132), the level splitting, i.e. the difference between the eigenenergies of even and odd states with here \( q_0 = 2n + 1, n = 0, 1, 2, \ldots \), for finite \( h^2 \), can be given by
\[
\Delta E(q_0, h^2) \approx \frac{4}{\pi} \left(\frac{\partial E}{\partial q}\right) \frac{y^{(l,z_0)}_{\text{WKB}}(0)}{y^{(l,z_0)}_{\text{WKB}}(0)}
\]
\[
= \frac{2}{\pi} \left(\frac{\partial E}{\partial (n + \frac{1}{2})}\right) \frac{y^{(l,z_0)}_{\text{WKB}}(0)}{y^{(l,z_0)}_{\text{WKB}}(0)} . \quad (147)
\]

In Ref. [18] the WKB level splitting is effectively (i.e. in the WKB restricted sense) defined by
\[
\Delta_{\text{WKB}} n = \frac{1}{\pi} \frac{\partial E}{\partial (n + \frac{1}{2})} \frac{y^{(l,z_0)}_{\text{WKB}}(0)}{y^{(l,z_0)}_{\text{WKB}}(0)} = \frac{1}{2} \Delta E(q_0, h^2) . \quad (148)
\]

Here \( \partial E/\partial n \) corresponds to the usual oscillator frequency. The result (146) is in Ref. [18] described as the “modified well and barrier” result \( \Delta_{n}^{\text{MWB}} \), the pure WKB result of Ref. [16] (i.e. that without the use of Stirling’s formula and so left in terms of \( e \) and \( n^n \)) being this divided by the Furry factor
\[
\text{f}_n := \left[ \frac{1}{2\pi} \left(\frac{e^n}{n + \frac{1}{2}}\right) \right]^{-1} ,
\]

\footnote{In Ref. [18] the “usual WKB approximation” of this expression is — with replacements \( h^4/4 \leftrightarrow k, c^2/2 \leftrightarrow \lambda \) — given as
\[
E_0 = -\frac{k^2}{4\lambda} + (2k)^{1/2} q - \frac{3\lambda}{4k} q^2 ,
\]
i.e. the following expression for large \( q \sim 2n + 1 \), which evidently supplies some correction terms.}
which is unity for $n \to \infty$ with Stirling’s formula.\footnote{Ref. [21], Eq. (66).} Of course, these derivations do not exploit the symmetry of the original equation under the interchanges $q \leftrightarrow -q$, $h^2 \leftrightarrow -h^2$, as we do here. We see therefore, that if this symmetry is taken into account from the very beginning (with the appropriate use of the Stirling formula) the Furry factor corrected result follows automatically. The Furry factor represents effectively a correction factor to the normalisation constants of WKB wave functions (which are normally $1/\sqrt{2\pi}$ and independent of $n$ as explained in Ref. [21]) to yield an improvement of WKB results for small values of $n$, as is also explained in Ref. [18].\footnote{Comparing the present work with that of Ref. [18], we identify the parameter $k$ there with $h^4/4$ here, and $\lambda$ there with $c^2/2$ here. Then the splitting $\Delta_{n}^{\text{MWB}}$ of Eq. (24) there is

\begin{align*}
\Delta_{n}^{\text{MWB}} &= \sqrt{\frac{1}{n!}} \frac{2^{10n+13}}{\sqrt{n!}} \left( \frac{h^6}{\sqrt{2\pi}} \right)^{n+1/2} \exp \left[ -\frac{\sqrt{2} k^{3/2}}{\lambda} \right] \\
&= \frac{h^2}{\sqrt{2\pi n!}} \frac{2^{2n+5}}{\sqrt{n!}} \left( \frac{h^6}{c^2} \right)^{n+1/2} \exp \left[ -\frac{h^6}{6\sqrt{2}c^2} \right]
\end{align*}

in agreement with $\Delta E(q_0, h^2)/2$ of Eq. (146).}

Had we taken the mass $m_0$ of the particle in the symmetric double-well potential equal to 1 (instead of 1/2), we would have obtained the result with $E$, $h^4$ and $c^2$ replaced by $2E$, $2h^4$ and $2c^2$ respectively (see Eq. (3)). Then

\begin{equation}
E(q_0, h^2) = E_0(q_0, h^2) \mp \frac{2^{q_0 + \frac{1}{2}} h^2 (\frac{h^6}{\sqrt{2\pi}})^{q_0/2}}{\sqrt{\pi} 2^{q_0/4} 4^{1/2} (q_0 - 1)!} e^{-\frac{h^6}{6\pi}}, \quad (149)
\end{equation}

and $\Delta E$ becomes

\begin{equation}
\triangle_1 E(q_0, h^2) \simeq 2^{q_0} \sqrt{\frac{2}{\pi}} \frac{h^2}{2^{q_0/4} (q_0 - 1)!} \left( \frac{h^6}{2^{1/2} c^2} \right)^{q_0/2} e^{-h^6/6c^2}, \quad (m_0 = 1)
\end{equation}

with

\begin{equation}
E_0(q_0, h^2)|_{m_0=1} = -\frac{h^8}{24c^2} + q_0 h^2 - \cdots.
\end{equation}

If in addition the potential is written in the form

\begin{equation}
V(z) = \frac{\lambda}{4} \left( z^2 - \frac{\mu^2}{\lambda} \right)^2, \quad \lambda > 0,
\end{equation}

\begin{equation}
\Delta_{n}^{\text{MWB}} = \sqrt{\frac{1}{n!}} \frac{2^{10n+13}}{\sqrt{n!}} \left( \frac{h^6}{\sqrt{2\pi}} \right)^{n+1/2} \exp \left[ -\frac{\sqrt{2} k^{3/2}}{\lambda} \right].
\end{equation}
a form frequently used in field theoretic applications, so that by comparison with Eq. (150) $h^4 \equiv 2\mu^2, c^2 = \lambda/2$, the level splitting is

$$\triangle_1 E(q_0, h^2) \simeq \frac{2^{q_0+2}\mu}{\pi^{1/2}2^{q_0+4}\frac{1}{2}(q_0 - 1)!!} \left( \frac{4\mu^3}{\lambda} \right)^{q_0/2} e^{-8^{1/2}\mu^3/3\lambda}. \quad (152)$$

This result agrees with the ground state $(n = 0)$ result of Ref. [9] using the path-integral method for the evaluation of pseudoparticle (instanton) contributions. Equation (150) agrees also with the result of Ref. [10] for arbitrary levels obtained with the use of periodic instantons† and with the results of Ref. [14] using multi-instanton methods‡.

5 Concluding Remarks

In the above we have presented a fairly complete treatment of the large-$h^2$ case of the quartic anharmonic oscillator, carried out along the lines of the corresponding calculations for the cosine potential and thus of the well-established Mathieu equation. In principle one could also consider the case of small values of $h^2$ and obtain convergent instead of asymptotic expansions; however, these are presumably not of much interest in physics. We considered only the symmetric two-minima potential. The asymmetric case can presumably also be dealt with in a similar way since various references point out that the asymmetric double well case can be transformed into a symmetric one (see e.g. Refs. [1], [14], [16]).

Every now and then literature appears which purports to overcome the allegedly ill-natured “divergent perturbation series” of the anharmonic oscillator problem, and reasons and even numerical studies are presented to support this claim. [30] It is clear — as also demonstrated by the work of Bender and Wu [1], [2] — that the expansions considered above are asymptotic. Tables of properties of Special Functions are filled with such expansions derived

---

*See Ref. [1], formula (4.11). The definition as $\triangle_n^{WKB}$ is used, so that the result of Eq. (150) differs by the factor 2 in Eq. (152).

†To help the comparison note that in Ref. [10] the potential is written as

$$V(z) = \eta^2 \left[ z^2 - \frac{m^2}{\eta^2} \right]$$

for $m_0 = 1$. The comparison with Eq. (150) therefore implies the correspondence $\eta^2 \leftrightarrow \lambda/2, m^2 \leftrightarrow \mu^2/2$, and $g^2$ is given as $g^2 = \eta^2/m^3$.

‡Ref. [14], first paper, Eqs. (2.34) and (E.15).
from differential equations for all the well-known and less well-known Special Functions. There is no reason to view the anharmonic oscillator solutions differently. In fact, in principle the Schrödinger equation of the quartic oscillator is an equation akin to equations like the Mathieu or modified Mathieu equations which lie outside the range of equations of hypergeometric type. The immense amount of literature meanwhile accumulated for instance in the case of the Mathieu equation can indicate what else can be achieved along parallel lines in the case of special types of Schrödinger equations, like that for anharmonic oscillators. Conversely, new methods discovered for dealing with the quartic oscillator could similarly be applied to the periodic potential and tested there.

The ground state splitting of the symmetric double well potential has been considered in a countless number of investigations. A reasonable, though incomplete list of references in this direction has been given by Garg \[31\] beginning with the well-known though nonexplicit (and hence not really useful) ground state formula in the book of Landau and Lifshitz \[32\]. Very illuminating discussions of double-wells and periodic potentials, mostly in connection with instantons, can be found in an article by Coleman \[33\]. The wide publicity given to the work of Bender and Wu \[2, 3\] made pure mathematicians aware of the subject; as some relevant references with their approach we cite Refs. \[34, 35, 36, 37, 38, 39\]. The double-well potential, in both symmetric and asymmetric form, has also been the subject of numerous numerical studies. As references in this direction, though not exclusively numerical, we cite papers of the Uppsala group \[40\]. Perturbation theoretical aspects have also been employed in Ref. \[41\]. Wave functions of symmetric and asymmetric double-well potentials have been considered in Ref. \[42\], in which it is demonstrated that actual physical tunneling takes place only into those states which have significant overlap with the false vacuum eigenfunction.

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Appendices

A Calculation of eigenvalues with the solutions of type A (inverted double well)

Here we use the solutions of type A, i.e. (20a), (20b), to obtain in leading order the eigenvalues $E$, i.e.

$$E(q, h^2) = \frac{1}{2} q h^2 + \frac{\triangle}{2 h^4}, \quad \triangle = -\frac{3}{2} c^2 (q^2 + 1) + O\left(\frac{1}{h^6}\right). \quad (A.1)$$

We rewrite the upper of Eqs. (13) in the following form with power expansion of the square root quantities and division by $h^2$:

$$-z A'(z) + \frac{1}{2} (q - 1) A(z)$$

$$= -\frac{1}{h^2} A''(z) - \frac{\triangle}{2 h^6} A(z) + \sum_{i=1}^{\infty} \left(\frac{2 c^2 z^2}{h^4}\right)^i \left[\alpha_i z A'(z) + \frac{1}{2} \beta_i A(z)\right], \quad (A.2)$$

where the expansion coefficients are given by

$$\alpha_0 = 1, \quad \alpha_1 = -\frac{1}{2}, \quad \alpha_2 = -\frac{1}{8}, \quad \alpha_3 = -\frac{1}{16}, \quad \alpha_4 = -\frac{5}{128}, \ldots,$$

$$\beta_0 = 1, \quad \beta_1 = -\frac{3}{2}, \quad \beta_2 = -\frac{5}{8}, \quad \beta_3 = -\frac{7}{16}, \ldots.$$

Using Eqs. (17) and (18) we obtain

$$A'_q(z) = \frac{1}{2} (q - 1) A_q(z) = \frac{1}{2} (q - 1) A_{q-2}(z)$$

and

$$A''_q(z) = \left[\frac{1}{2} (q - 1)\right]^2 \frac{1}{z} A_q(z) - \frac{1}{2} (q - 1) A_{q-2}(z)$$

$$= \frac{1}{4} (q - 1)(q - 3) A_{q-4}(z). \quad (A.3)$$
The lowest order solution $A^{(0)} = A_q(z)$ therefore leaves uncompensated on the right hand side of the equation for $A$ the terms amounting to

$$R_q^{(0)} = -\frac{1}{4h^2}(q-1)(q-3)A_{q-4} - \frac{\Delta}{2h^6}A_q - \frac{c^2}{2h^4}(q+2)A_{q+4} - \left(\frac{c^2}{2h^4}\right)^2(q+4)A_{q+8} + \frac{1}{2} \sum_{i=3}^{\infty} \left(\frac{2c^2z^2}{h^4}\right)^i [ (q-1)\alpha_i + \beta_i ] A_q.$$ 

Clearly one now uses the relation

$$z^{2i} A_q(z) = A_{q+4i}(z).$$

In this way $R_q^{(0)}$ is expressed as a linear combination of functions $A_{q+4i}(z)$. As always in the procedure, one observes that

$$D_q := -z\frac{d}{dz} + \frac{1}{2}(q-1), \quad D_{q+4i} = D_q + 2i, \quad D_q\frac{\mu A_{q+4i}}{-2i} = \mu A_{q+4i}. \quad \text{(A.4)}$$

Thus a term $\mu A_{q+4i}$ in $R_q^{(0)}$ can be taken care of by adding to $A^{(0)}$ the contribution $\frac{\mu A_{q+4i}}{-2i}$ except, of course, when $i = 0$. In this way we obtain the next order contribution $A^{(1)}$ to $A^{(0)}$ and the coefficient of terms with $i = 0$, i.e. those in $A_q(z)$, give an equation from which $\Delta$ is determined. Hence in the present case

$$A^{(1)} = -\frac{1}{4h^2}(q-1)(q-3)A_{q-4} - \frac{c^2}{2h^4}(q+2)A_{q+4} - \left(\frac{c^2}{2h^4}\right)^2(q+4)\frac{A_{q+8}}{-4} + \cdots. \quad \text{(A.5)}$$

In its turn $A^{(1)}$ leaves uncompensated terms amounting to

$$R_q^{(1)} = -\frac{1}{4h^2}(q-1)(q-3)\frac{1}{2} \left\{ \left( -\frac{1}{4h^2} \right)(q-5)(q-7)A_{q-8} - \frac{c^2}{2h^4}A_q - \frac{\Delta}{2h^6}A_{q-4} - \left(\frac{2c^2}{h^4}\right)^2\frac{q}{16}A_{q+4} + \cdots \right\}$$

$$-\frac{c^2}{2h^4}(q+2) \left\{ -\frac{1}{4h^2}(q+3)(q+1)A_q - \frac{c^2}{2h^4}(q+6)A_{q+8} - \frac{\Delta}{2h^6}A_{q+4} + \cdots \right\} + \cdots.$$
The sum of terms with $A_q$ in $R_q^{(0)}, R_q^{(1)}, \ldots$ must then be set equal to zero. Hence to the order we are calculating here

\[
0 = \frac{c^2}{(4h^2)(4h^4)}[(q - 1)(q - 2)(q - 3) - (q + 1)(q + 2)(q + 3)] + \mathcal{O}\left(\frac{1}{h^6}\right) - \frac{\triangle}{2h^6},
\]

(A.6)

i.e.

\[
0 = -\frac{c^2}{2^6 h^6} 12(q^2 + 1) - \frac{\triangle}{2h^6} + \mathcal{O}\left(\frac{1}{h^6}\right).
\]

It follows that

\[
\triangle = -\frac{3}{2}c^2(q^2 + 1) + \mathcal{O}\left(\frac{1}{h^6}\right).
\]

The same result is obtained in connection with the solution of type $B$, as explained in the text.

## B Evaluation of $y_B(0), \overline{y}_C(0), y_B'(0), \overline{y}_C'(0)$

We show that — with $w = h z$ — the leading terms of the quantities listed are given by

\[
B_q(0) = \frac{1}{\sqrt{\pi}} \frac{[\frac{1}{4}(q - 3)]! \sin\left\{\frac{\pi}{4}(q + 1)\right\}}{[\frac{1}{4}(q - 1)]! \sin\left\{\frac{\pi}{4}(q + 1)\right\}},
\]

\[
\overline{C}_q(0) = \frac{\sqrt{\pi}}{\left[-\frac{1}{4}(q + 1)\right]! \left[\frac{1}{4}(q - 1)\right]!},
\]

\[
\left[\frac{d}{dw} B_q(w)\right]_0 = -\sqrt{\frac{2}{\pi}} \sin\left\{\frac{\pi}{4}(q + 3)\right\},
\]

\[
\left[\frac{d}{dw} \overline{C}_q(w)\right]_0 = i\frac{2}{\pi} \sin\left\{\frac{\pi}{4}(q - 3)\right\}.
\]

(B.1a)

In fact, with the reflection formula $(-z)!(z - 1)! = \pi/\sin \pi z$, one finds that

\[
\left[-\frac{1}{4}(q + 1)\right]! = \frac{\pi}{[\frac{1}{4}(q - 3)]! \sin\left\{\frac{\pi}{4}(q + 1)\right\}} \quad \text{and hence} \quad \frac{B_q(0)}{\overline{C}_q(0)} = 1.
\]

(B.1b)
From the literature, e.g. Ref. [25], we obtain
\[ D_{\frac{1}{2}(q-1)}(0) = \frac{\sqrt{\pi}}{2^{\frac{1}{2}}(q-1)!} \left( -\frac{1}{4}(q + 1) \right)! \]
\[ D_{\frac{1}{2}(q+1)}(0) = -\frac{\sqrt{\pi}}{2^{\frac{1}{2}}(q+1)!} \left( -\frac{1}{4}(q + 3) \right)! \]  \hspace{0.5cm} (B.2)

Thus with the help of the reflection formula cited above:
\[ B_q(0) = \frac{D_{\frac{1}{2}(q-1)}(0)}{\left[ \frac{1}{4}(q - 1)! \right] 2^{\frac{1}{2}}(q-1)!} = \frac{\sqrt{\pi}}{\left[ \frac{1}{4}(q - 1)! \right] 2^{\frac{1}{2}}(q-1)!} \]
\[ = \frac{1}{\sqrt{\pi}} \frac{\left[ \frac{1}{4}(q - 3)! \right]}{\left[ \frac{1}{4}(q - 1)! \right]!} \sin \left( \frac{\pi}{4} \right) \]
\[ = \frac{1}{\sqrt{\pi}} \frac{\left[ \frac{1}{4}(q - 3)! \right]}{\left[ \frac{1}{4}(q - 1)! \right]!} \sin \left( \frac{\pi}{4} \right) \]  \hspace{0.5cm} (B.3)

Expressions for \( C_q(0), [C'_q(w)]_{w=0} \) follow with the help of the "circuit relation" of parabolic cylinder functions given in the literature as
\[ D_{\frac{1}{2}(q-1)}(w) = e^{-\frac{i\pi}{2} (q-1)} D_{\frac{1}{2}(q-1)}(-w) \]
\[ + \frac{\sqrt{2\pi} e^{-\frac{i\pi}{4} (q+1)}}{\left[ -\frac{1}{4}(q + 1)! \right]!} D_{-\frac{1}{2}(q+1)}(-iw). \]

From this relation we obtain
\[ D_{-\frac{1}{2}(q+1)}(0) = \sqrt{\frac{\pi}{2}} \frac{D_{\frac{1}{2}(q-1)}(0)}{\left[ \frac{1}{4}(q - 1)! \right]! \cos \left( \frac{\pi}{4} (q - 1) \right) \}. \]

Inserting from \( \text{(B.2)} \), using the above reflection formula and the duplication formula \( \sqrt{\pi}(2z)! = 2^{2z} z!(z - 1/2)! \), we obtain
\[ D_{-\frac{1}{2}(q+1)}(0) = \frac{\sqrt{\pi}}{2^{\frac{1}{2}(q+1)}(-\frac{1}{4}(q + 1)!)}. \]

From this we derive
\[ C_q(0) = \frac{D_{-\frac{1}{2}(q+1)}(0)}{2^{-\frac{1}{2}(q+1)}(-\frac{1}{4}(q + 1)!) \left[ -\frac{1}{4}(q + 1)! \right]!} \]
\[ = \frac{\left[ \frac{1}{4}(q - 3)! \right]}{\sqrt{\pi} \left[ \frac{1}{4}(q - 1)! \right]!} \sin \left( \frac{\pi}{4} \right) \]  \hspace{0.5cm} (B.5)
Similarly we obtain

\[ [D_{\frac{1}{2}(q+1)}'(iw)]_{w=0} = \frac{-i\sqrt{\pi}}{2^{\frac{1}{2}(q-1)}[\frac{1}{4}(q-3)]!} \]  \hspace{1cm} (B.6)

and

\[ [C_q'(w)]_0 = \frac{D_{\frac{1}{2}(q+1)}(0)}{[-\frac{1}{4}(q+1)]!2^{-\frac{1}{2}(q+1)} = \frac{-i\sqrt{2\pi}}{[-\frac{1}{4}(q+1)]![\frac{1}{4}(q-3)]!} \]

\[ = -i\sqrt{\frac{2}{\pi}} \sin\left\{\frac{\pi}{4}(q+1)\right\} = i\sqrt{\frac{2}{\pi}} \sin\left\{\frac{\pi}{4}(q-3)\right\}. \]  \hspace{1cm} (B.7)

C Calculation of eigenvalues with solutions of type A (double well)

We show in conjunction with the derivation of solution \(y_A\) that the leading terms of \(\triangle\) and hence \(E\) are given by

\[ \triangle = -c^2(3q^2 + 1) - \frac{\sqrt{2}c^4}{4h^6} q(17q^2 + 19) + \cdots, \]

\[ E(q, h^2) = -\frac{h^8}{2^8c^2} + \frac{1}{\sqrt{2}} qh^2 - \frac{c^2(3q^2 + 1)}{2h^4} \]

\[ -\sqrt{2}c^4 q(17q^2 + 19) + O\left(\frac{1}{h^{16}}\right). \]  \hspace{1cm} (C.1)

The structure of the solution \(93\) for \(A_q(z)\) is very similar to that of the corresponding solution in considerations of other potentials, such as periodic potentials. Thus it is natural to explore analogous steps. The first such step would be to reexpress the right hand side of Eq. \(91a\) with \(A_q\) replaced by \(A_q\) as a linear combination of terms \(A_{q+2i}, i = 0, \pm 1, \pm 2, \ldots\). First, however, we reexpress \(A''_q\) in terms of functions of \(z\) multiplied by \(A_q\). We know the first derivative of \(A_q\) from Eq. \(92\), i.e.

\[ A'_q(z) = \frac{qz_+ - z}{z^2 - z_+^2} A_q(z). \]  \hspace{1cm} (C.2)
Differentiation yields

\[ A''_q(z) = \frac{A_q(z)}{(z^2 - z^2_+)^2} \left[ (z - qz_+)^2 - (z^2 - z^2_+) + 2z(z - qz_+) \right] \]

\[ = \frac{A_q(z)}{(z^2 - z^2_+)^2} \left[ 2z^2 - 4zz_+q + z^2_+(q^2 + 1) \right]. \quad \text{(C.3)} \]

We wish to rewrite this expression as a sum

\[ \sum_i \text{coefficient}_i A_q + 2^i (\frac{z}{z^2 - z^2_+})^i. \]

We also note at this stage the derivative of the entire solution \( y_A(z) \) taking into account only the dominant contribution:

\[ y'_A(z) \approx \left[ \frac{c}{\sqrt{2}}(z^2 - z^2_+) + (qz_+ - z) \right] A_q(z) \exp \left[ \frac{1}{\sqrt{2}} \left( \frac{c}{3} z^3 - \frac{h^4}{4c} z \right) \right]. \quad \text{(C.4)} \]

We observe some properties of the function \( A_q(z) \) given by Eq. (93):

\[ A_{q+2i}A_{q+2j} = A_{q+2i+2j}A_q, \quad \frac{A_{q+2}}{A_q} = \frac{z - z_+}{z + z_+} = \frac{A_q}{A_{q-2}}, \quad \text{(C.5)} \]

\[ \frac{A_{q+2} + A_{q-2}}{A_q} = 2\frac{z^2 + z^2_+}{z^2 - z^2_+}, \quad \frac{A_{q+2} - A_{q-2}}{A_q} = -4\frac{z_+}{z^2 - z^2_+}, \quad \text{(C.6)} \]

\[ \frac{(A_{q+2} - A_{q-2})^2}{A_q} = \left( 4zz_+ \right)^2 \left( \frac{A_q}{(z^2 - z^2_+)^2} \right)^2 = A_{q+4} - 2A_q + A_{q-4}, \quad \text{(C.7)} \]

From these we obtain, for instance by componendo et dividendo,

\[ -\frac{z}{z_+} = \frac{A_{q+2} + A_q}{A_{q+2} - A_q} \]

\[ = - \left( 1 + \frac{A_{q+2}}{A_q} \right) \left[ 1 + \left( \frac{A_{q+2}}{A_q} \right) + \left( \frac{A_{q+2}}{A_q} \right)^2 + \cdots \right] \]

\[ = - \left[ 1 + 2\frac{A_{q+2}}{A_q} + 2\frac{A_{q+4}}{A_q} + 2\frac{A_{q+6}}{A_q} + \cdots \right]. \quad \text{(C.8)} \]

Similarly we obtain

\[ -\frac{z_+}{z} = \frac{A_{q+2} - A_q}{A_{q+2} + A_q} \]

\[ = - \left[ 1 - 2\frac{A_{q+2}}{A_q} + 2\frac{A_{q+4}}{A_q} - 2\frac{A_{q+6}}{A_q} + \cdots \right]. \quad \text{(C.9a)} \]
and from this
\[ \frac{z^2}{z^2} = 1 - 4\frac{A_{q+2}}{A_q} + 8\frac{A_{q+4}}{A_q} - 12\frac{A_{q+6}}{A_q} + 16\frac{A_{q+8}}{A_q} - \cdots. \] (C.9b)

Hence with Eq. (C.7)

\[
\frac{z}{(z^2 - z^2_+)^2} A_q = \frac{z_+}{z_+ z^2} \left( \frac{1}{4z_+} \right)^2 [A_{q+4} - 2A_q + A_{q-4}]
= \frac{1}{z_+} \left( \frac{1}{4z_+} \right)^2 [A_{q+4} - 2A_q + A_{q-4}] \left[ 1 - 2\frac{A_{q+2}}{A_q} + 2\frac{A_{q+4}}{A_q} - \cdots \right]
= \frac{1}{z_+} \left( \frac{1}{4z_+} \right)^2 [A_{q-4} - 2A_{q-2} + 0 + 2A_{q+2} - A_{q+4} + \cdots].
\] (C.10)

Finally with Eqs. (C.7) and (C.9b) we obtain

\[
\frac{A_q}{(z^2 - z^2_+)^2} = \frac{z^2 A_q}{(z^2 - z^2_+)^2} \frac{1}{z^2} = \left( \frac{1}{4z_+} \right)^2 [A_{q+4} - 2A_q + A_{q-4}] \frac{1}{z_+^2} \left[ 1 - 4\frac{A_{q+2}}{A_q} + 8\frac{A_{q+4}}{A_q} - 12\frac{A_{q+6}}{A_q} + \cdots \right]
= \left( \frac{1}{2z_+} \right)^4 [A_{q-4} - 4A_{q-2} + 6A_q - 4A_{q+2} + A_{q+4} + \cdots].
\] (C.11)

Inserting expressions (C.7), (C.10) and (C.11) into Eq. (C.3), we obtain*

\[
A''_q = \left( \frac{1}{4z_+} \right)^2 [(q - 1)(q - 3)A_{q-4} - 4(q - 1)^2A_{q-2} + 2(3q^2 + 1)A_q
- 4(q + 1)^2A_{q+2} + (q + 1)(q + 3)A_{q+4} + \cdots].
\] (C.12)

Hence the first approximation of \( A \),

\[ A^{(0)} = A_q, \]

*The reader may observe the similarity with the corresponding coefficients in the simpler case of the cosine potential, cf. Ref. [5]. Infinite series like here for solutions of type \( A \) arise in the more complicated cases, e.g. in the corresponding treatment of the elliptic potential (Lamé equation); cf. Ref. [27].
leaves uncompensated on the right hand side of Eq. (91a) the contribution

\[
R_q^{(0)} = -\frac{\sqrt{2}}{2c} \left[ A''_q + \frac{\Delta}{h^4} A_q \right]
\]

\[
= -\frac{\sqrt{2}c}{2^3 h^4} [(q, q - 4) A_{q-4} + (q, q - 2) A_{q-2} + (q, q) A_q + (q, q + 2) A_{q+2} + (q, q + 4) A_{q+4} + (q, q + 6) A_{q+6} + \cdots],
\]

where the lowest coefficients have been determined above as

\[
(q, q \pm 4) = (q \mp 1)(q \mp 3), \quad (q, q \mp 2) = -4(q \mp 1)^2, \quad (q, q) = 2(3q^2 + 1) + 16z^2 \frac{\Delta}{h^4} = 2(3q^2 + 1) + \frac{2}{c^2} \Delta.
\]

It is now clear how the calculation of higher order contributions proceeds in our standard way. In particular the dominant approximation of \(\Delta\) is obtained by setting \((q, q) = 0\), i.e.

\[
\Delta = -c^2(3q^2 + 1),
\]

\[
E(q, h^2) = -\frac{h^8}{2^5 c^2} + \frac{1}{\sqrt{2}} q h^2 - \frac{c^2(3q^2 + 1)}{2h^4} + O\left(\frac{1}{h^6}\right).
\]

Since

\[
\mathcal{D}_q A_q = 0, \quad \mathcal{D}_{q+2i} A_{q+2i} = 0 \quad \text{and} \quad \mathcal{D}_{q+2i} = \mathcal{D}_q + 2iz_+,
\]

we have

\[
\mathcal{D}_q \left( \frac{A_{q+2i}}{-2i z_+} \right) = A_{q+2i},
\]

except, of course, for \(i = 0\). The first approximation \(A^{(0)} = A_q\) leaves uncompensated on the right hand side of Eq. (91a) the contribution \(R_q^{(0)}\). Terms \(\mu A_{q+2i}\) in this may therefore be eliminated by adding to \(A^{(0)}\) the contribution \(A^{(1)}\) given by

\[
A^{(1)} = \left( -\frac{\sqrt{2}c}{2^3 h^4} \right) \left[ \frac{(q, q - 4) A_{q-4}}{8 z_+} + \frac{(q, q - 2) A_{q-2}}{4 z_+} \right. \left. + \frac{(q, q + 2)}{-4 z_+} A_{q+2} + \frac{(q, q + 4)}{-8 z_+} A_{q+4} + \cdots \right].
\]
The sum \( A = A^{(0)} + A^{(1)} \) then represents a solution to that order provided the sum of terms in \( A_q \) in \( R_q^{(0)} \) and \( R_q^{(1)} \) is set equal to zero, where \( R_q^{(1)} \) is the sum of terms left uncompensated by \( A^{(1)} \), i.e.

\[
R_q^{(1)} = \left( -\frac{\sqrt{2}c}{2^3h^4} \right) \left( \frac{(q,q-4)}{8z_+} R_q^{(0)} + \frac{(q,q-2)}{4z_+} R_{q-2}^{(0)} + \cdots \right). \tag{C.16}
\]

This coefficient of \( A_q \) set equal to zero yields to that order the following equation

\[
0 = \left( -\frac{\sqrt{2}c}{2^3h^4} \right) (q,q) + \left( -\frac{\sqrt{2}c}{2^3h^4} \right)^2 \left( \frac{(q,q-4)(q-4,q)}{8z_+} \right.
\]
\[
+ \frac{(q,q-2)(q-2,q)}{4z_+} \left. \right) + \frac{(q,q+2)(q+2,q)}{-4z_+}
\]
\[
+ \frac{(q,q+4)(q+4,q)}{-8z_+} \right] + \cdots ,
\]

which reduces to

\[
0 = 2(3q^2 + 1) + \frac{2}{c^2} \Delta + \frac{\sqrt{2}c^2}{2h^6} q(17q^2 + 19), \tag{C.17}
\]

thus yielding the next approximation of \( \Delta \).

\section*{D Calculation of eigenvalues with solutions of type B (double well)}

Equation (C.11) or (C.17) can also be obtained in conjunction with the solutions of types B or C. The initial step is to use the recurrence relation of parabolic cylinder functions \( D_{\nu}(w) \) to reexpress the right hand side of Eq. (83a) as a linear combination of functions \( B_q(w) \) defined by Eq. (98a). Thus with the recurrence relation

\[
w D_{\nu}(w) = D_{\nu+1}(w) + \nu D_{\nu-1}(w) \tag{D.1}
\]

and the expression (98a), i.e.

\[
B_q(w) = \frac{D_{\frac{1}{2}(q-1)}(w)}{\left[ \frac{1}{4}(q-1) \right]! 2^{\frac{1}{4}}(q-1)^{\frac{1}{4}}}, \tag{D.2}
\]
we obtain

\[ wB_q(w) = \sqrt{2} \left[ \frac{1}{4} (q + 1) \right]! B_{q+2} + \left[ \frac{1}{4} (q - 3) \right]! B_{q-2}. \] (D.3)

The procedure is then similar to that in the case of the solution of type A.

E Recalculation of tunneling deviation using WKB solutions

Here we determine the tunneling deviation \( q - q_0 \) of \( q \) from an odd integer \( q_0 \), above obtained as Eq. (116), by now using the periodic WKB solutions below the turning points.

The turning points at \( z_0 \) and \( z_1 \) on either side of the minimum at \( z_+ \) are given by Eqs. (119) and (120). We start from Eq. (131), i.e.

\[ y_\pm(z) = \frac{1}{2} \left[ y_A(z) \pm y_{\text{WKB}}^{(l,z_0)}(z) \right] = \frac{1}{2\gamma} y_{\text{WKB}}^{(l,z_0)}(z) \pm \frac{1}{2\gamma} y^{(r,z_0)}_{\text{WKB}}(z). \] (E.1)

Different from above we now continue the solutions (in the sense of linearly matched WKB solutions) across the turning point at \( z_0 \) in the direction of the minimum of the potential at \( z_+ \). Then ((r, z_0) meaning to the right of \( z_0 \) and note the asymmetric factor of 2)\(^\dagger\)

\[
\begin{align*}
y_\pm(z) & = \frac{1}{2\gamma} y^{(r,z_0)}_{\text{WKB}}(z) \pm \frac{1}{2\gamma} y^{(r,z_0)}_{\text{WKB}}(z) = \left[ \frac{1}{2} qh^2 - \frac{1}{4} h^4 U(z) \right]^{-1/4} \\
& \times \left\{ \frac{1}{\gamma} \sin \left[ \int_{z_0}^z dz \left( \frac{1}{2} qh^2 - \frac{1}{4} h^4 U(z) \right)^{1/2} + \frac{\pi}{4} \right] \right. \\
& \pm \frac{1}{\gamma} \cos \left[ \int_{z_0}^z dz \left( \frac{1}{2} qh^2 - \frac{1}{4} h^4 U(z) \right)^{1/2} + \frac{\pi}{4} \right] \right\}. \tag{E.2}
\end{align*}
\]

\(^\dagger\)See Ref. [22], p. 291, Eqs. (21), (22) or Ref. [26], Vol. I, Sec. 6.2.4.
We also note that
\[
\frac{d}{dz} y_{\pm}(z) \simeq \left[ \frac{1}{2} q h^2_{+} - \frac{1}{4} h^4_{+} U(z) \right]^{1/4}
\times \left\{ \frac{1}{\gamma} \cos \left[ \int_{z_0}^{z} dz \left( \frac{1}{2} q h^2_{+} - \frac{1}{4} h^4_{+} U(z) \right)^{1/2} + \frac{\pi}{4} \right] \right.
\left. \mp \frac{1}{\gamma} \sin \left[ \int_{z_0}^{z} dz \left( \frac{1}{2} q h^2_{+} - \frac{1}{4} h^4_{+} U(z) \right)^{1/2} + \frac{\pi}{4} \right] \right\}. \tag{E.3}
\]

We now apply the boundary conditions (105) and (106) at the minimum \(z_+\) and obtain the conditions:
\[
0 = \frac{2}{\gamma} \sin \left[ \int_{z_0}^{z_+} dz \left( \frac{1}{2} q h^2_{+} - \frac{1}{4} h^4_{+} U(z) \right)^{1/2} + \frac{\pi}{4} \right] \]
\[
\quad \mp \frac{1}{\gamma} \cos \left[ \int_{z_0}^{z_+} dz \left( \frac{1}{2} q h^2_{+} - \frac{1}{4} h^4_{+} U(z) \right)^{1/2} + \frac{\pi}{4} \right]. \tag{E.4}
\]

and
\[
0 = \frac{2}{\gamma} \cos \left[ \int_{z_0}^{z_+} dz \left( \frac{1}{2} q h^2_{+} - \frac{1}{4} h^4_{+} U(z) \right)^{1/2} + \frac{\pi}{4} \right] \]
\[
\quad \mp \frac{1}{\gamma} \sin \left[ \int_{z_0}^{z_+} dz \left( \frac{1}{2} q h^2_{+} - \frac{1}{4} h^4_{+} U(z) \right)^{1/2} + \frac{\pi}{4} \right]. \tag{E.5}
\]

Hence
\[
\tan \left[ \int_{z_0}^{z_+} dz \left( \frac{1}{2} q h^2_{+} - \frac{1}{4} h^4_{+} U(z) \right)^{1/2} + \frac{\pi}{4} \right] \simeq \mp \frac{\gamma}{2\gamma} \tag{E.6}
\]
and
\[
\cot \left[ \int_{z_0}^{z_+} dz \left( \frac{1}{2} q h^2_{+} - \frac{1}{4} h^4_{+} U(z) \right)^{1/2} + \frac{\pi}{4} \right] \simeq \pm \frac{\gamma}{2\gamma} \tag{E.7}
\]

In the present considerations we approach the minimum of the potential at \(z_+\) by coming from the left, i.e. from \(z_0\). We could, of course, approach the minimum also from the right, i.e. from \(z_1\). Then at any point \(z \in (z_0, z_1)\) we expect\(^\dagger\)
\[
|y_{\text{WKB}}^{(r, z_0)}(z)| = |y_{\text{WKB}}^{(l, z_1)}(z)|, \quad |y_{\text{WKB}}^{(r, z_0)}(z)| = |y_{\text{WKB}}^{(l, z_1)}(z)|. \tag{E.8}
\]
\(^\dagger\)See e.g. Ref. [26], Sec. 6.2.6.
Choosing the point \( z \) to be \( z_+ \), this implies
\[
\left| \frac{\sin}{\cos} \left( \int_{z_0}^{z_+} dz \left[ \frac{1}{2} q h_+^2 - \frac{1}{4} h_+^4 U(z) \right]^{1/2} + \frac{\pi}{4} \right) \right| = \left| \frac{\sin}{\cos} \left( \int_{z_0}^{z_1} dz \left[ \frac{1}{2} q h_+^2 - \frac{1}{4} h_+^4 U(z) \right]^{1/2} + \frac{\pi}{4} \right) \right|. \tag{E.9}
\]
Thus e.g.
\[
\cos \left[ \int_{z_0}^{z_1} dz \left( \frac{1}{2} q h_+^2 - \frac{1}{4} h_+^4 U(z) \right)^{1/2} + \frac{\pi}{4} \right] = \cos \left[ \int_{z_0}^{z_1} \cdots - \frac{\pi}{4} + \int_{z_0}^{z_1} + \frac{\pi}{4} \right] = \cos \left[ \int_{z_0}^{z_1} \cdots - \frac{\pi}{4} - \int_{z_0}^{z_1} + \frac{\pi}{4} \right] = \cos \left[ \int_{z_0}^{z_1} \cdots + \frac{\pi}{4} \right]
\]
provided the Bohr–Sommerfeld–Wilson quantisation condition holds, i.e.
\[
\int_{z_0}^{z_1} dz \left( \frac{1}{2} q h_+^2 - \frac{1}{4} h_+^4 U(z) \right)^{1/2} = (2n + 1) \frac{\pi}{2}, \quad n = 0, 1, 2, 3, \ldots, \tag{E.10}
\]
where it is understood that (cf. Eq. (83))
\[
\frac{1}{2} q h_+^2 \simeq E - V(z_\pm).
\]

Similarly under the same condition
\[
\sin \left[ \int_{z_+}^{z_1} \cdots + \frac{\pi}{4} \right] = (-1)^n \sin \left[ \int_{z_0}^{z_+} \cdots + \frac{\pi}{4} \right].
\]

We rewrite the quantisation condition in the present context and in view of the symmetry of the potential in the immediate vicinity of \( z_+ \) as half that of Eq. (E.10), i.e.
\[
\int_{z_0}^{z_+} dz \left( \frac{1}{2} q h_+^2 - \frac{1}{4} h_+^4 U(z) \right)^{1/2} \simeq q \frac{\pi}{4}. \tag{E.11}
\]
The integral on the left can be approximated by
\[
\frac{h_+^2}{2} \int_{z_0}^{z_+} dz \left( \frac{2q}{h_+^2} - (z - z_+)^2 \right)^{1/2} = \frac{q}{2} \sin^{-1} \frac{z_+ - z_0}{(2q/h_+^2)^{1/2}} = \frac{q}{4} \pi
\]
in agreement with the right hand side (the last step following from Eqs. [119] and [120]). We now see that Eqs. [E.6] and [E.7] assume a form as in our perturbation theory, i.e. they become

\[ \tan \left\{ (q + 1) \frac{\pi}{4} \right\} \simeq \mp \frac{\gamma}{2\gamma}, \quad \cot \left\{ (q + 1) \frac{\pi}{4} \right\} \simeq \mp \frac{\gamma}{2\gamma}. \]  

(E.12)

The equations corresponding to these in Ref. [18] are there described as WKB quantisation conditions of the double minimum potential. Since

\[ \tan \left\{ (q + 1) \frac{\pi}{4} \right\} = 0 \quad \text{for} \quad q = q_0 = 3, 7, 11, \ldots, \]

\[ \cot \left\{ (q + 1) \frac{\pi}{4} \right\} = 0 \quad \text{for} \quad q = q_0 = 1, 5, 9, \ldots, \]  

(E.13)

we can expand the left hand sides about these points and thus obtain

\[ q - q_0 \simeq \pm \frac{2\gamma}{\pi \gamma} \]  

\[ \mp 4 \sqrt{\frac{1}{2\pi} \left[ \frac{1}{2} \left( \frac{h_z^2}{2} \right) \right] \left( \frac{\gamma_0}{2\gamma} \right)^2 \left( 2z_+ \right)^{\gamma_0} e^{-\frac{1}{2} h_z^2 z_+^2} \]  

for \( q_0 = 1, 3, 5, \ldots \)  

(E.14)

in agreement with Eq. (116). We note here incidentally that this agreement demonstrates the significance of the factor of 2 in the first equality of Eq. (E.14) which results from the factor of 2 in front of the sine in the WKB formula (E.2).

**F Evaluation of WKB exponential with elliptic integral**

Here we evaluate the elliptic integral \( I_2(0) \) of Eq. (135a).

**F.1 Parameters and their expansions**

The expression to be evaluated is

\[ I_2 = \frac{2}{3G^2} (1 + u)^{1/2} \left[ E(k) - uK(k) \right]. \]  

(F.1)

We have

\[ k^2 = \frac{1 - u}{1 + u}, \quad u = G \sqrt{2q}, \quad q \simeq 2n + 1. \]  

(F.2)
Hence we obtain for $G$ close to zero:

$$k^2 = \frac{1 - G\sqrt{2q}}{1 + G\sqrt{2q}} = 1 - 2G\sqrt{2q} + 4G^2q - \cdots, \quad k^2 \sim 1, \quad (F.3)$$

and

$$(1 + u)^{1/2} = (1 + G\sqrt{2q})^{1/2} = 1 + G\sqrt{\frac{q}{2}} - \frac{G^2q}{4} - \cdots, \quad (F.4)$$

and

$$k'^2 = 1 - k^2 = 2G\sqrt{2q} - 4G^2q + \cdots, \quad k'^2 \sim 0. \quad (F.5)$$

We now reexpress various quantities in terms of $u$. Thus

$$k'^2 = 2u - 2u^2 + \cdots, \quad (F.6)$$

and hence

$$k' = \sqrt{2u(1 - u)^{1/2}} = \sqrt{2u(1 - \frac{u}{2} + \cdots)}. \quad (F.7)$$

The following expression appears frequently in the expansions of elliptic integrals. Therefore it is convenient to deal with this here. We have

$$\frac{4}{k'} = \frac{4}{\sqrt{2u(1 - \frac{u}{2} + \cdots)}} = \frac{4}{\sqrt{2u}} \left(1 + \frac{u}{2} + \cdots\right). \quad (F.8)$$

Hence

$$\ln\left(\frac{4}{k'}\right) = \ln\left[\frac{4}{\sqrt{2u}}\left(1 + \frac{u}{2} - \cdots\right)\right] \simeq \ln\left(\frac{4}{\sqrt{2u}}\right) + \frac{u}{2}. \quad (F.9)$$

### F.2 Evaluation of elliptic integrals

Our next objective is the evaluation of the elliptic integrals $E(k)$ and $K(k)$ by expanding these in ascending powers of $k'^2$, which is assumed to be small. We obtain the expansions from Ref. [29] as

$$E(k) = 1 + \frac{1}{2} \left[\ln\left(\frac{4}{k'}\right) - \frac{1}{2}\right]k'^2 + \frac{3}{16} \left[\ln\left(\frac{4}{k'}\right) - \frac{13}{12}\right]k'^4 + \cdots \quad (F.10)$$

and

$$K(k) = \ln\left(\frac{4}{k'}\right) + \frac{1}{4} \left[\ln\left(\frac{4}{k'}\right) - 1\right]k'^2 + \cdots. \quad (F.11)$$
Consider first \( E(k) \):

\[
E(k) = 1 + \frac{1}{2} \left[ \ln \left( \frac{4}{\sqrt{2u}} \right) + \frac{u}{2} - \frac{1}{2} \right] 2u(1-u) \\
+ \frac{3}{16} \left[ \ln \left( \frac{4}{\sqrt{2u}} \right) + \frac{u}{2} - \frac{13}{12} \right] 4u^2(1-u)^2 + \cdots \\
= 1 + \ln \left( \frac{4}{\sqrt{2u}} \right) \left\{ u(1-u) + \frac{3}{4} u^2(1-u)^2 \right\} \\
+ \frac{1}{2} (u-1)u(1-u) + \frac{1}{12} \left( u - \frac{13}{6} \right) u^2(1-u)^2 + \cdots
\]

We can rewrite this as

\[
E(k) = 1 + \ln \left( \frac{4}{\sqrt{2u}} \right) \frac{u(1-u)}{4} \left\{ 4 + 3u(1-u) \right\} \\
+ \frac{1}{243} u(u-1)(1-u) \{24 - 3u(6u-13)\}. \quad (F.12)
\]

Analogously we have

\[
uK(k) = u \left[ \ln \left( \frac{4}{\sqrt{2u}} \right) + \frac{u}{2} \right] + \frac{u}{4} \left[ \ln \left( \frac{4}{\sqrt{2u}} \right) + \frac{u}{2} - 1 \right] 2u(1-u) \\
= \ln \left( \frac{4}{\sqrt{2u}} \right) \left\{ u + \frac{1}{2} u^2(1-u) \right\} + \frac{1}{2} u^2 \left[ 1 + (1-u) \left( \frac{u}{2} - 1 \right) \right] \\
= \ln \left( \frac{4}{\sqrt{2u}} \right) \frac{1}{2} u^2(1-u) + 2u \right\} + \frac{1}{4} u^2 \left[ 2 + (1-u)(u-2) \right]
\]

or

\[
uK(k) = \ln \left( \frac{4}{\sqrt{2u}} \right) \frac{u}{2} \left\{ u(1-u) + 2 \right\} + \frac{1}{4} u^2 \left[-u^2 + 3u \right] \\
= \ln \left( \frac{4}{\sqrt{2u}} \right) \frac{u}{2} \left\{ u(1-u) + 2 \right\} - \frac{1}{4} u^3(u - 3). \quad (F.13)
\]
With (F.12) and (F.13) we obtain

$$E(k) - uK(k)$$

$$= 1 + \ln \left( \frac{4}{\sqrt{2u}} \right) \left[ \frac{1}{4} u(1-u)\{4 + 3u(1-u)\} - \frac{1}{2} u\{u(1-u) + 2\} \right]$$

$$+ \frac{1}{2} u(u - 1)(1 - u) \frac{1}{2^{4/3}} \{24 - 3u(6u - 13)\} + \frac{1}{4} \ u^3(u - 3)$$

$$= 1 + \ln \left( \frac{4}{\sqrt{2u}} \right) \frac{u}{4} [1 - u] \{4 + 3u(1-u)\} - 2\{u(1-u) + 2\}]$$

$$+ \frac{1}{2.46} u(u - 1)(1 - u)\{24 - 3u(6u - 13)\} + \frac{1}{4} u^3(u - 3). \quad (F.14)$$

Now consider the last line here without the factor 2.46 in the denominator and in the last step pick out the lowest order terms in $u$ (i.e. up to and including $u^2$):

$$u(u - 1)(1 - u)\{24 - 3u(6u - 13)\} + 12u^3(u - 3)$$

$$= -u(1 - u)^2\{24 - 18u^2 + 39u\} + 12u^3(u - 3)$$

$$= -3u(1 - u)^2\{8 - 6u^2 + 13u\} + 12u^3(u - 3)$$

$$\simeq -3u.8 + 6u^2.8 - 3.13u^2$$

$$= -3u.8 + 9u^2. \quad (F.15)$$

Now consider the bracket $[\ldots]$ in (F.14), i.e.

$$[(1 - u)\{4 + 3u(1-u)\} - 2\{u(1-u) + 2\}] = u(3u^2 - 4u - 3). \quad (F.16)$$

From (F.13) with (F.14) and (F.15) we now obtain

$$E(k) - uK(k) \simeq 1 + \ln \left( \frac{4}{\sqrt{2u}} \right) \frac{1}{4} u^2(3u^2 - 4u - 3) - \frac{1}{2} u + \frac{9u^2}{2.46}. \quad (F.17)$$

### F.3 Evaluation of $I_2$

We now return to Eq. (F.1), i.e.

$$I_2 = \frac{2}{3G^2} (1 + u)^{1/2}[E(k) - uK(k)].$$
Inserting here from the above expansions the contributions up to and including those of order \( u^2 \), we obtain:

\[
I_2 \approx \frac{2}{3G^2} \left( 1 + \frac{u}{2} - \frac{1}{8} u^2 + \cdots \right) \left[ 1 - \ln \left( \frac{4}{\sqrt{2}} \right) \frac{u^2}{4} (3 + 4u - 3u^2) \right.
\]
\[
- \frac{1}{2} u + \frac{3u^2}{16} + O(u^3) \Bigg] .
\]  

(F.18)

Remembering that \( u = G \sqrt{2q} \), this becomes

\[
I_2 \approx \frac{2}{3G^2} - \frac{u^2}{2G^2} \ln \left( \frac{4}{\sqrt{2}} \right) + \frac{2}{3G^2} \left( - \frac{3u^2}{8} \right) + \frac{u^2}{8G^2}
\]
\[
= \frac{2}{3G^2} - q \ln \left( \frac{2^{1/2} G^{1/2} 2^{1/4} q^{1/4}}{} \right) - \frac{q}{4}
\]
\[
= \frac{2}{3G^2} - \frac{q}{2} \ln \left( \frac{2^{5/2}}{G q^{1/2}} \right) - \frac{q}{4} .
\]  

(F.19)

Thus

\[
I_2 \approx \frac{2}{3G^2} + \frac{q}{2} \ln \left( \frac{G}{4} \right) - \frac{q}{4} \ln \left( \frac{2}{q} \right) - \frac{q}{4}
\]
\[
= \frac{2}{3G^2} + \frac{1}{2} (2n + 1) \ln \left( \frac{G}{4} \right) + \frac{1}{4} (2n + 1) \ln \left( \frac{2n + 1}{2} \right)
\]
\[
- \left( \frac{2n + 1}{4} \right) .
\]  

(F.20)