Application of the discrete WKB method to spin tunneling

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Abstract

A discrete version of the WKB method is developed and applied to calculate the tunnel splittings between classically degenerate states of spin Hamiltonians. The results for particular model problems are in complete accord with those previously found using instanton methods. The discrete WKB method is more elementary and also yields wavefunctions.

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I. INTRODUCTION

A large variety of problems in physics can be modeled in terms of a spin of large magnitude which is then described by a Hamiltonian which is a polynomial in the spin components. It is natural in many of these cases to seek a semiclassical description. This is especially so when the system possesses a number of degenerate states in the classical limit, and one wishes to see how this degeneracy is lifted by quantum tunneling. Examples include the Lipkin-Meshov-Glick model in nuclear physics [1,2], the rotational spectrum of polyatomic molecules [3], and the Hamamoto-Mottleson model [4] for the $\Delta I = 4$ staggering of the rotational spectra of certain superdeformed nuclei.

Perhaps the simplest example of such a problem is provided by the Hamiltonian

$$\mathcal{H} = -k_1 S_z^2 + k_2 S_x^2,$$

where $k_1 > 0$, $k_2 > 0$, and $S_\alpha$ ($\alpha = x, y, z$) are components of the spin operator $\mathbf{S}$ obeying the usual commutation rules

$$[S_\alpha, S_\beta] = i\epsilon_{\alpha\beta\gamma} S_\gamma.$$  \hspace{1cm} (1.2)

Further, the spin has a magnitude $S$, i.e., the operator $\mathbf{S} \cdot \mathbf{S}$ has eigenvalue $S(S + 1)$. As $S \to \infty$, the system is more and more classical, and in the limit it has two degenerate ground states corresponding to $S_z/S = \pm 1$. For large but finite $S$, the quantal analogs of these states will be admixed by a tunneling matrix element $\Delta_0/2$. The two lowest energy eigenstates will then be split by an amount $\Delta_0$. The goal of a tunneling calculation is to find an expression for $\Delta_0$ that is asymptotically valid as $S \to \infty$. In analogy with the result for particles with a position like coordinate in a potential well, we expect this expression to take the form

$$\Delta_0 = e^{-(B_0 + B_1 + B_2 + \cdots)},$$  \hspace{1cm} (1.3)

where

$$B_0 \gg B_1 \gg B_2 \gg \cdots$$ \hspace{1cm} (1.4)

in the sense that $B_1/B_0, B_2/B_1, \ldots \to 0$ as $S \to \infty$. By looking at the commutation relations for the scaled operators $S_\alpha/S$, we can see that $1/S$ plays the same role as $\hbar$ in conventional WKB theory, and we thus expect $B_0 = O(S)$. As is often done for a particle in a well, it is convenient to call $e^{-B_0}$ the Gamow factor, or the WKB exponent, and the remaining terms $e^{-(B_1 + B_2 + \cdots)}$ the prefactor.

In many physical problems, it is only sensible or possible to calculate $\Delta_0$ to “exponential accuracy”, i.e., to find only the leading term $B_0$ in Eq. (1.3). As a general point of formalism, however, it is clearly desirable to have a proper asymptotic approximation $\Delta_0'$ to $\Delta_0$ itself and not just to $\ln \Delta_0$. In other words, we demand that $\Delta_0'/\Delta_0 \to 1$ as $S \to \infty$. For this one must know all $B_n$ that are of $O(S^0)$ or greater. The first correct calculation to such accuracy that we know of was done by Enz and Schilling [5,6], who mapped the spin onto a canonically conjugate variable pair via a Villain transformation, and then applied an instanton method [7] to the resulting problem. Great care must be taken in this approach...
with operator ordering problems, leading to a rather complex calculation. A more natural approach is one based on Klauder’s spin-coherent-state path integral [9]. A naive application of instanton methods for the tunnel splitting to this path integral [10], however, only gives the leading $S$ dependence correctly. In particular, terms of $O(S^0)$ in $\ln \Delta_0$ are incorrectly obtained [11,12]. A correct calculation within this formalism has only recently been done by Belinicher, Providencia, and Providencia [13], who show that it is necessary to consider non-differentiable paths by a careful examination of the discrete time version of the path integral. Once again, the simplicity of the instanton approach is lost.

It is therefore desirable to have a means of calculating the tunnel splitting using only elementary methods of analysis. Such an approach is provided by the discrete WKB method. (An alternative approach, used in Ref. [14], also meets the criterion of being elementary.) In the present context, the method consists of writing the Schrödinger equation as a recursion relation for the expansion coefficients of an energy eigenstate in the $S_z$ basis, and solving this recursion relation under the assumption that the coefficients in the recursion relation vary slowly with $m$, the $S_z$ eigenvalue. By and large, the method is a straightforward generalization of the continuous WKB method [15], and it may also be viewed as equivalent to the use of semiclassical dynamics for Bloch electrons.

The earliest appearance of this method in a physics context of which we are aware is by Schulten and Gordon [16], who use it to find semiclassical approximations for the $3j$ (Wigner) and $6j$ (Racah) symbols. A cogent review of the method in the context of atomic physics has been given by Braun [17], who also cites its application in a variety of other physics settings, as well as earlier discussions in Russian mathematics texts. It has also been previously applied to spin tunneling problems by van Hemmen and Sütő [18,19]. These authors have not, however, utilized the method to its full potential. Specifically, they calculate $\Delta_0$ for a class of Hamiltonians including

$$\mathcal{H} = -\gamma S_z^2 - \alpha S_x,$$

but only the leading $S$ dependence is correctly found. One of the goals of this paper is to show that the prefactor can also be found correctly to order $S^0$ with little extra labor. (See Sec. V.)

We will illustrate the discrete WKB method by applying it to Eqs. (1.1) and (1.5). We will find the splittings $\Delta_k$, $k = 0, 1, 2, \ldots$ for all low lying pairs of energy levels for Eq. (1.4), and the lowest splitting $\Delta_0$ for Eq. (1.3). Our answers for $\Delta_0$ agree completely with those of Enz and Schilling [7], or Belinicher, Providencia, and Providencia [13], and we believe they are obtained with much less effort. While the discrete WKB method does not have the nice geometrical structure of the spin-coherent-state path integral approach, it provides compensation in that it yields wavefunctions in the course of the calculation, which may be of further use; for evaluating matrix elements of perturbations, for example [20,21]. Other problems commonly solved by the continuous WKB method, such as escape from a metastable well, are also amenable to the method, but we do not discuss these here.

The plan of the paper is as follows. In Sec. II we briefly review the discrete WKB method. Our discussion is heuristic and physically motivated. See Braun [17] for one that is more formal. In Sec. III we derive a formula [see Eq. (3.11)] for the tunnel splitting for a symmetric double well problem analogous to that for the continuous case [22,23]. We apply the method to the Hamiltonian (1.1) in Sec. IV, and to (1.5) in Sec. V. We compare our
answers for the splittings with numerical results, and in the case of Eq. (1.3) to answers given by van Hemmen and Sütő [19], and Scharf, Wreszinski, and van Hemmen [14].

II. THE DISCRETE WKB METHOD

To introduce the discrete WKB method, let us consider the Hamiltonian (1.1), and focus on an energy eigenfunction $|\psi\rangle$. Denoting $S_z$ eigenfunctions $|m\rangle$ with $S_z|m\rangle = m|m\rangle$ as usual, and writing $C_m = \langle m|\psi\rangle$, it is easy to see that Schrödinger’s equation takes the form of a three-term recursion relation connecting $C_{m-2}$, $C_m$, and $C_{m+2}$. The step $\Delta m = 2$ in the index is inconvenient, so it is preferable to change the notation somewhat, and relabel the states which are connected to each other by an index $j$, with $j = 1, 2, \ldots, N$, where $N$ equals $S$ or $S + 1$. The Schrödinger equation then takes the form

$$w_j C_j + t_{j,j+1} C_{j+1} + t_{j,j-1} C_{j-1} = EC_j,$$

where $w_j = \mathcal{H}_{jj}$ and $t_{j,j+1} = \mathcal{H}_{j,j+1}$, with $t_{N,N+1}$ and $t_{N+1,N}$ being understood as zero. We may also assume that $t_{j,j+1} \neq 0$ for any $j$, since otherwise the matrix for $\mathcal{H}$ is block diagonal, and Eq. (2.1) may be regarded as applying to one block. We can also choose the phases of the basis states so that all $t_{j,j+1}$ are real. Hermiticity then yields $t_{j+1,j} = t^*_{j,j+1} = t_{j,j+1}$.

The above problem is equivalent to a tight-binding model for an electron on a one-dimensional lattice with on-site energies $w_j$, and hopping matrix elements $t_{j,j+1}$, and indeed our notation is chosen to reflect this analogy. If $w_j$ and $t_{j,j+1}$ vary slowly enough with $j$ (how slowly will be seen below) we may use the approximation of semiclassical electron dynamics. To do this we first note that for the uniform case where $w_j = w$ and $t_{j,j+1} = t$ for all $j$, the eigenstates are Bloch states with wavefunction $e^{i q j}$ and energy $E(q) = w + 2t \cos q$. For the nonuniform case, we first extend $j$ to be a continuous variable, and define $w(j)$ and $t(j)$ to be extensions of $w_j$ and $t_{j,j+1}$ via the relations

$$w(j) = w_j,$$

$$t(j) = (t_{j,j+1} + t_{j,j-1}) / 2,$$

which are required to hold whenever $j$ is an integer. We further demand that $w(j)$ and $t(j)$ be smooth enough that if $j/N$ is regarded as a quantity of order $N^0$, then

$$\frac{dw}{dj} = O \left( \frac{w(j)}{N} \right),$$

and likewise for $t(j)$. This equation is the formal statement of ‘slowly varying’ coefficients. Whether or not it can be satisfied depends, of course, on the problem under consideration, and it is this condition which determines whether or not the problem is amenable to solution by the discrete WKB method. It is easy to see that it holds for Eq. (1.1) whenever $S \gg 1$.

We next define a local wavevector $q(j)$ by the relation

$$\cos q(j) = (E - w(j)) / 2t(j).$$

Further, since the electron velocity is given by $\partial E / \partial q$ in semiclassical dynamics, we define
Then by a straightforward repeat of the arguments employed in the continuous WKB method (see [15], e.g.), it is a simple matter to show that two linearly independent solutions to Eq. (1.1) are given by

\[ C_j \sim \frac{1}{\sqrt{v(j)}} \exp \left( \pm i \int q(j')dj' \right). \]

A general solution is obtained by taking linear combinations of these two solutions.

A formal proof of Eq. (2.7) is given by Braun [17], along with connection formulas, Bohr-Sommerfeld quantization rules, etc. We will therefore limit ourselves to a few key comments and comparisons with the continuous WKB method.

The first point is that Eq. (2.7) represents a development of \( \log C_j \) in powers of \( N^{-1} \), in which only the leading two terms are kept. To this accuracy, we need only keep the first two terms of \( w(j) \) and \( t(j) \) in an expansion in powers of \( 1/N \). Alternatively, we can use any expression for these functions which will reproduce the first two terms correctly. In particular, Eqs. (2.2) and (2.3) need only hold to this order. In considering this point, it should be remembered that \( j/N \) is regarded as being of \( O(1) \).

The second point is that the factor \( 1/\sqrt{v} \) in Eq. (2.7) has the effect of normalizing each of the two solutions so that the probability flux is conserved and has a value of unity. This follows from noting that \( |C_j|^2 \sim 1/v \), so that the particle spends a time inversely proportional to its velocity in any given coordinate segment \( dj \). Since this is exactly what we expect for a classical particle, the quantum mechanical wavefunction is correctly adjusted to give a conserved probability flux.

The third point is that for a given energy \( E \), the classically accessible region of motion is defined by the inequalities

\[ U^-(j) \leq E \leq U^+(j), \]

where

\[ U^\pm = w(j) \pm 2|t(j)|. \]

This follows from Eqs. (2.5) and (2.6) because whenever the condition (2.8) is violated, \( q(j) \) and \( v(j) \) acquire imaginary parts. The expression (2.7) [with \( \sqrt{v(j)} \) replaced by \( \sqrt{|v(j)|} \) as usual] then describes an exponentially decaying or growing wavefunction as opposed to an oscillatory one. It may also be noted that for uniform \( w_j \) and \( t_{j, j \pm 1} \), the quantities \( U^\pm \) would be the limits of the allowable range of Bloch state energies. More generally they may be regarded as local, \( j \)-dependent band edges.

Finally, let us note the conditions for the validity of Eq. (2.7). The physical requirement is that the wavelength of the particle should not change by very much over dimensions of the wavelength itself, which is equivalent to demanding that

\[ |dq(j)/dj| \ll \sin^2 q(j). \]

In addition to failing if \( w(j) \) and \( t(j) \) do not vary slowly (as defined above), it is easy to see that Eq. (2.10) is violated whenever \( q \approx 0 \) or \( \pm \pi \). In light of Eqs. (2.8) and (2.9), this is hardly surprising, since these are turning points of the classical motion. Solutions of the form (2.7) on opposite sides of these points must be related to each other by the above mentioned connection formulas, as in the usual WKB method.
III. GENERAL FORMULA FOR TUNNEL SPLITTING

In this section we consider the problem where the functions \( w_j \) and \( t_{j,j+1} \) possess reflection symmetry about some point, and the central region is classically forbidden for some energies. The band-edge functions \( U^\pm(j) \) then have the form shown in Fig. 1. We will derive a formula [see Eq. (3.11)] for the tunnel splitting between states formed from symmetrical states localized in the two potential wells. Our approach is completely analogous to that for a continuous coordinate \[22\]. Except for the extension to odd and even numbers of sites, essentially the same derivation also appears in Ref. \[24\], and a formula very close to Eq. (3.11) also appears in van Hemmen and Wreszinski \[23\]. Our notation is sufficiently different, and the argument sufficiently brief, that it is worth giving it in toto.

It is convenient to shift the index \( j \) so that it runs over the values 
\[-\frac{N-1}{2}, -\frac{N-3}{2}, \ldots, \frac{N-1}{2}\].

(3.1)

Note that \( j \) takes on integer values when \( N \) is odd, and half-integer values when \( N \) is even. With this labelling, we have
\[ t_{j,k} = t_{-k,-j} = t_{k,j}. \]

(3.2)

It is also convenient, for future use, to define \( j_0 = 1 \) or \( 1/2 \), depending on whether \( N \) is odd or even, respectively. In either case, \( j_0 \) labels the first site to the right of the mid-point. We also define \( J = (N-1)/2 \), and \( t_{\text{mid}} = t_{10} \) or \( t_{1/2,-1/2} \) for odd or even \( N \).

Let \( C_j \) be the normalized wavefunction localized in the right well, and which satisfies the Schrödinger equation (2.1), neglecting the possibility of tunneling, with some energy \( E_0 \). Further, let \( a_j \) and \( s_j \) be the exact associated antisymmetric and symmetric wavefunctions, respectively, and let them have energies \( E_1 \) and \( E_2 \), where \( (E_1+E_2)/2 = E_0 \). These functions are given to very good accuracy by
\[ a_j = \frac{1}{\sqrt{2}}(C_j - C_{-j}), \]
\[ s_j = \frac{1}{\sqrt{2}}(C_j + C_{-j}). \]

(3.3)

Since the product \( C_jC_{-j} \) is everywhere exponentially small, these functions are properly normalized to unity.

The Schrödinger equations obeyed by \( C_j \) and \( a_j \) are
\[ (w_j - E_0)C_j + t_{j,j-1}C_{j-1} + t_{j,j+1}C_{j+1} = 0, \]
\[ (w_j - E_1)a_j + t_{j,j-1}a_{j-1} + t_{j,j+1}a_{j+1} = 0. \]

(3.4)

(3.5)

We multiply Eq. (3.4) by \( a_j \), Eq. (3.5) by \( C_j \), subtract the latter from the former, and sum the result from \( j = j_0 \) to \( J \equiv (N-1)/2 \). This yields
\[ (E_1 - E_0) \sum_{j \geq j_0} C_j a_j + \Sigma_1 - \Sigma_2 = 0, \]

(3.6)

where
\[
\Sigma_1 = \sum_{j \geq j_0} a_j(t_{j,j-1}C_{j-1} + t_{j,j+1}C_{j+1}), \quad (3.7)
\]
\[
\Sigma_2 = \sum_{j \geq j_0} C_j(t_{j,j-1}a_{j-1} + t_{j,j+1}a_{j+1}). \quad (3.8)
\]

By shifting the index of summation in Eq. (3.8) we can see that most of the terms in the sums \( \Sigma_1 \) and \( \Sigma_2 \) are identical. Recalling that \( t_{j,j+1} = 0 \), and that \( a_0 = 0 \) for odd \( N \), we obtain

\[
\Sigma_1 - \Sigma_2 = \begin{cases} a_1 t_{\text{mid}} C_0 & (\text{odd } N); \\ a_{1/2} t_{\text{mid}} (C_{1/2} + C_{-1/2}) & (\text{even } N). \end{cases} \quad (3.9)
\]

To evaluate the sum \( \sum_j a_jC_j \) in Eq. (3.6), we use Eq. (3.3). Since \( C_{-j} \) is exponentially small everywhere in the right hand well, and since \( C_j \) is normalized,

\[
\sum_{j \geq j_0} C_ja_j \approx \frac{1}{\sqrt{2}} \sum_{j \geq j_0} C_j^2 = \frac{1}{\sqrt{2}}. \quad (3.10)
\]

Substituting Eqs. (3.3), (3.9), and (3.10) in Eq. (3.6), and recalling that \( E_1 - E_2 = 2(E_1 - E_0) \), we obtain

\[
E_1 - E_2 = \begin{cases} -2 t_{\text{mid}} C_0(C_1 - C_{-1}) & (\text{odd } N); \\ -2 t_{\text{mid}} (C_{1/2}^2 - C_{-1/2}^2) & (\text{even } N). \end{cases} \quad (3.11)
\]

Equation (3.11) is the sought for formula for the splitting. Note that unlike the case of a particle with a continuous coordinate degree of freedom, it is not now necessary for the antisymmetric state to have the higher energy. In fact, it is not hard to show that

\[
\text{sgn} (E_1 - E_2) = \begin{cases} 1 & (\text{odd } N); \\ -\text{sgn } t & (\text{even } N). \end{cases} \quad (3.12)
\]

### IV. TUNNEL SPLITTINGS FOR MODEL HAMILTONIAN (1.1)

We now apply our general formalism to the Hamiltonian (1.1). Writing a general eigenstate of \( \mathcal{H} \) as

\[
|\psi\rangle = \sum_m C_m |m\rangle, \quad (4.1)
\]

where \( S_z|m\rangle = m|m\rangle \), Schrödinger’s equation becomes

\[
(w_m - E)C_m + t_{m,m+2}C_{m+2} + t_{m,m-2}C_{m-2} = 0, \quad (4.2)
\]

with

\[
w_m = (k_1 + \frac{1}{2}k_2)(S(S + 1) - m^2), \quad (4.3)
\]
\[
t_{m,m+2} = \frac{1}{4}k_2[(S(S + 1) - m(m + 1))(S(S + 1) - (m + 1)(m + 2))]^{1/2}. \quad (4.4)
\]
For convenience, we have added a constant $k_1S(S + 1)$ to the Hamiltonian, and thus to $w_m$.

As noted earlier, Eq. (4.2) is of the same form as Eq. (2.1) with the minor difference that the index $m$ jumps in steps of 2 rather than 1. We can take care of this point by changing the integral in the exponential in Eq. (2.7) to $\int q(m')dm'/2$, leaving the other formulas unaffected.

One elementary point should be noted at this stage. For half-integer $S$, Kramers’ theorem ensures an exact double degeneracy of all energy eigenstates of the Hamiltonian (1.1). This means that $\Delta_k$ vanishes. In the spin-coherent-state path integral approach, this result comes about because the kinetic term in the action is a Berry phase, and different symmetry related paths acquire phases which give rise to destructive interference for half-integer $S$. In the discrete WKB method, this result comes about from an almost trivial separation of the eigenvalue problem into two isomorphic disjoint subspaces.

There are two steps in the calculation of $\Delta_k$ via Eq. (3.11). First, one must find the wavefunction $C_m$ in the classically allowed and disallowed regions separately. In the present case, an expression for the former can be found exactly and in such a way that it actually holds in part of the disallowed region. This allows one to match on to the quasiclassical wavefunction given by Eq. (2.7) without using connection formulas. The second step consists of substituting the quasiclassical wavefunction into Eq. (3.11).

To execute the first step, let us consider a wavefunction $C^{(k)}_m$ with energy $E^{(k)}_m$ which corresponds to the $k$th state localized in the well near $m = -S$, and begin by finding it near this well. The coefficients $w_m$ and $t_{m,m+2}$ are evaluated by writing $m = -S + n$, and expanding Eqs. (4.3) and (4.4) in powers of $1/S$, with $n$ regarded as a quantity of order $S^0$. This yields

$$w_{-S+n} = (k_1 + \frac{1}{2}k_2)(2n + 1)S,$$  \hspace{1cm} (4.5)

$$t_{-S+n,-S+n+2} = \frac{1}{2}k_2S((n + 1)(n + 2))^{1/2}.$$  \hspace{1cm} (4.6)

Rewriting $C_{-S+n} = b_n$, the recursion relation (4.2) reads

$$(2k_1 + k_2)(n + \frac{1}{2})b_n + \frac{1}{2}k_2S\sqrt{n(n + 1)}b_{n-2} + \frac{1}{2}k_2S\sqrt{(n + 1)(n + 2)}b_{n+2} = Eb_n,$$  \hspace{1cm} (4.7)

which is immediately recognizable as arising from the harmonic oscillator Hamiltonian

$$H_{osc} = (2k_1 + k_2)S\left(a^\dagger a + \frac{1}{2}\right) + \frac{1}{2}k_2S\left(a^2 + (a^\dagger)^2\right),$$  \hspace{1cm} (4.8)

where $a$ and $a^\dagger$ are the annihilation and creation operators obeying $[a, a^\dagger] = 1$. To see this let us denote the $k$th energy state of $H_{osc}$ by $|\psi_k\rangle$, and the number eigenstates by $|n\rangle$ with $a^\dagger a|n\rangle = n|n\rangle$. It is then apparent that $b^{(k)}_n = \langle n|\psi_k\rangle$ obeys the eigenvalue equation (4.7).

To find $b^{(k)}_n$, we transform to position and momentum operators $x$ and $p$ obeying $[x, p] = i$ via $a = (x + ip)/\sqrt{2}, a^\dagger = (x - ip)/\sqrt{2}$. In terms of these,

$$H_{osc} = \left(k_1 + \frac{1}{2}k_2\right)S(x^2 + p^2) + \frac{1}{2}k_2S(x^2 - p^2).$$  \hspace{1cm} (4.9)

It follows that the $k$th state $|\psi_k\rangle$ has an energy
\[ E_0^{(k)} = (k + \frac{1}{2}) \omega_0, \quad (4.10) \]
\[ \omega_0 = 2S(k_1(k_1 + k_2))^{1/2}. \quad (4.11) \]

The wavefunction of this state is given by a textbook formula:
\[ \langle x|\psi_k \rangle = \left(2^{2k}(k!)^2 \pi \xi^2\right)^{-1/4} e^{-x^2/2\xi^2} H_k(x/\xi), \quad (4.12) \]
where \( H_k \) is the \( k \)th Hermite polynomial, and
\[ \xi^2 = \left(\frac{k_1}{k_1 + k_2}\right)^{1/2} \equiv \tanh(\kappa/2). \quad (4.13) \]

It is also useful to write \( \xi = e^{-\theta} \), in terms of which we have the symmetrical relations
\[ e^{-2\theta} = \tanh(\kappa/2), \quad e^{-\kappa} = \tanh \theta. \quad (4.14) \]

The number states \(|n\rangle\) on the other hand, have wavefunctions
\[ \langle x|n \rangle = \left(2^{2n}(n!)^2 \pi\right)^{-1/4} e^{-x^2/2} H_n(x). \quad (4.15) \]

We can thus evaluate the overlap \( \langle n|\psi_k \rangle = b_n^{(k)} \) in the \( x \) representation. The requisite integrals are most simply found by using the generating function for the Hermite polynomials,
\[ e^{2xz - z^2} = \sum_{n=0}^{\infty} \frac{z^n}{n!} H_n(x). \quad (4.16) \]

The final result for \( b_n^{(k)} \) is
\[ b_n^{(k)} = \cos(\pi D) \left(\frac{n! k!}{2^{n+k} \cosh \theta}\right)^{1/2} \sum_{j=0}^{[k/2]} \frac{(-1)^j (\tanh \theta)^{D+2j} (2 \sech \theta)^{k-2j}}{(D+j)! (k-2j)! j!}. \quad (4.17) \]

Here \( D \equiv (n-k)/2 \), and \([x]\) denotes the largest integer less than or equal to \( x \). Note that the \( \cos(\pi D) \) factor accounts for the vanishing of \( b_n^{(k)} \) if \( n-k \) is odd. The latter fact is a simple consequence of the parity relation \( H_n(-x) = (-1)^n H_n(x) \). It can be seen as a restatement of the separation of \( \mathcal{H} \) into two subspaces, or of the \( \Delta m = 2 \) step in Eq. (4.2), and rigorously implies \( C_m^{(k)} = 0 \) for odd \( m + S - k \) for the entire range of \( m \).

Next, let us find \( C_m^{(k)} \) in the central or classically forbidden region where \( S - m \) and \( S + m \) are both \( O(S) \). In this region, we have to sufficient accuracy
\[ u(m) = \left(k_1 + \frac{1}{2}k_2\right) \left(S + \frac{1}{2}\right)^2 - m^2 + O(S^0), \quad (4.18) \]
\[ t(m) = \frac{1}{4} k_2 \left(S + \frac{1}{2}\right)^2 - m^2 + O(S^0). \quad (4.19) \]

It is easy to see that \( d(u/t)/dm = O(S^{-1}) \), so the quasiclassicality condition (2.10) holds if \( S \gg 1 \). Equation (2.5) then yields for the local wavevector
\[
\cos q(m) = \frac{2E_0^{(k)} - (2k_1 + k_2) \left((S + \frac{1}{2})^2 - m^2\right)}{k_2 \left((S + \frac{1}{2})^2 - m^2\right)}
\]
\[
= -\left(\frac{2k_1 + k_2}{k_2}\right) + \frac{2E_0^{(k)}}{k_2(2S + 1)} \left(\frac{1}{S + \frac{1}{2} - m} + \frac{1}{S + \frac{1}{2} + m}\right). \tag{4.20}
\]

For the discrete WKB method to work, the energy levels which are split must lie well below the barrier, i.e., \(E_0^{(k)} \ll (k_1 + k_2/2)S^2\). The second term in Eq. (4.20) is then of order \(S^{-1}\) relative to the first, and we can solve for \(q(m)\) as an expansion in powers of \(1/S\). Equation (4.13) implies that

\[
1 + 2k_1/k_2 = \cosh \kappa, \tag{4.21}
\]

so that

\[
q(m) = \pi + i \left[\kappa - \frac{E_0^{(k)}}{\omega_0} \left(\frac{1}{S + \frac{1}{2} - m} + \frac{1}{S + \frac{1}{2} + m}\right) + O\left(\frac{E_0^{(k)}}{\omega_0 S^2}\right)\right]. \tag{4.22}
\]

The exponent in Eq. (2.7) therefore equals (recalling the extra factor of \(1/2\) due to the step \(\Delta m = 2\))

\[
\phi(m) = i \int ^m q(m') \frac{dm'}{2} = \frac{i\pi m}{2} - \frac{\kappa m}{2} + \frac{E_0^{(k)}}{2\omega_0} \ln \left(\frac{S + \frac{1}{2} + m}{S + \frac{1}{2} - m}\right) + \cdots. \tag{4.23}
\]

Similarly, correct to leading order in \(S\), we have

\[
|v(m)| = \frac{\omega_0}{2S} \left((S + \frac{1}{2})^2 - m^2\right) \tag{4.24}
\]

We now substitute Eqs. (4.23) and (4.24) into Eq. (2.7), changing the normalization from unit flux to total unit probability in accord with the discussion in Sec. III. Writing the result only for the nonzero \(C_m^{(k)}\), i.e., for \(m + S - k\) even, we have

\[
C_m^{(k)} \approx A_k \frac{(S + \frac{1}{2} + m)^{(2k-1)/4}}{(S + \frac{1}{2} - m)^{(2k+3)/4}} e^{i\pi(m-k)/2} e^{-\kappa m/2}, \tag{4.25}
\]

where \(A_k\) is the normalization constant, and we have used \(E_0^{(k)}/\omega_0 = k + \frac{1}{2}\).

It is now possible to match Eqs. (4.25) and (4.17) directly, since both results are valid in the region \(S \gg n \gg 1\). We first find \(b_n^{(k)}\) for \(S \gg n \gg k\), with \(k = O(1)\):

\[
b_n^{(k)} = \frac{\cos(\pi(n - k)/2)}{\sqrt{k!}} \left(\frac{2}{\pi}\right)^{1/4} (\text{sech} \theta)^{(2k+1)/2} (\tanh \theta)^{(n-k)/2} n^{(2k-1)/4}. \tag{4.26}
\]

To find \(C_m^{(k)}\) in the overlap region, we put \(m = -S + n\) in Eq. (4.25), recall that \(e^{-\kappa} = \tanh \theta\), and in this way obtain for \(n \gg 1\),

\[
C_{-S+n}^{(k)} = \frac{A_k}{(2S)^{(2k+3)/4}} \cos(\pi(n-k)/2) e^{-i\pi S/2} (\tanh \theta)^{(n-S)/2} n^{(2k-1)/4}. \tag{4.27}
\]
Comparing with Eq. (4.26) we obtain

\[ A_k = e^{i\pi S/2} \left( \frac{2}{\pi} \right)^{1/4} \frac{1}{\sqrt{k!}} \left( \frac{\text{sech} \theta}{2k+1} \right)^{1/2} \left( \tanh \theta \right)^{1/2} \left( S-k \right)^{1/2} \left( 2S \right)^{1/4}. \]  

(4.28)

The last step is to apply Eq. (3.11) for the splitting. The only issue requiring caution is that of even versus odd \( N \), the number of points on which the wavefunction \( C^{(k)}_m \) is nonzero. We have \( N = S + 1 \) for even \( k \) and \( N = S \) for odd \( k \). Thus the parity of \( N \) is that of \( S + k - 1 \). Both cases can be easily handled at the same time, however. From Eq. (4.25), we see that for \( |m| \ll S \), the nonvanishing \( C^{(k)}_m \)'s are given by \( (A_k/S)e^{-\kappa m/2} \) up to an overall phase. Thus, the factor multiplying \( 2t_{\text{mid}} \) in Eq. (3.11) equals \( 2 \sinh \kappa |A_k/S|^2 \) in magnitude in both cases. Similarly, we see from Eq. (4.4) that \( t_{\text{mid}} \) equals \( k^2 S^2/4 \) in both cases. Thus,

\[ \Delta_k = k^2 \sinh \kappa |A_k|^2 \]  

(4.29)

for all \( k \) and \( S \).

It remains to substitute Eq. (4.28) into Eq. (4.29). We quote the answer in terms of the parameters \( \omega_0 \) and \( \theta \):

\[ \Delta_k = \frac{1}{k!} \left( \frac{4S}{\sinh 2\theta} \right)^k \Delta_0, \]  

(4.30)

\[ \Delta_0 = 4 \omega_0 \left( \frac{S}{\pi} \right)^{1/2} \text{sech} \theta (\tanh \theta)^S. \]  

(4.31)

For some purposes, it may be desirable to write these results in terms of the ratio \( \xi \) defined in Eq. (4.13). The conversion is easily done using the formulas

\[ \tanh \theta = (1 - \xi^2)/(1 + \xi^2), \]  

(4.32)

\[ \text{sech} \theta = 2\xi/(1 + \xi^2), \]  

(4.33)

\[ (1/\sinh 2\theta) = 2\xi/(1 - \xi^4). \]  

(4.34)

As mentioned before, the result (4.31) for the ground state splitting agrees with that of Enz and Schilling [7] and Belinicher, Providencia, and Providencia [13]. A comparison with numerically obtained exact answers is given in Table I. As is evident, the agreement is quite good, and improves with increasing \( S \).

The formula (4.30) for the higher splittings is, to our knowledge, new.

V. TUNNEL SPLITTING FOR MODEL HAMILTONIAN (1.5)

In this section we apply our method to the Hamiltonian (1.5), limiting ourselves to finding the ground state tunnel splitting \( \Delta_0 \). This time the recursion relation connects contiguous coefficients \( C_{m-1}, C_m, \) and \( C_{m+1} \), and

\[ w(m) = -\gamma m^2, \]  

(5.1)

\[ t(m) = (\alpha/2)(S'^2 - m^2)^{1/2}, \]  

(5.2)

where we have introduced the convenient abbreviation...
\[ S' = S + 1/2. \] (5.3)

Let us begin, as in the previous section, by finding the wavefunction for the state localized in the right hand well, \( C_m \), in the classically accessible region. This time the answer depends on how the parameters \( \alpha \) and \( \gamma \) are taken to vary as \( S \to \infty \). To see this note that the lower band-edge function \( U^-(m) \) now has a quadratic as opposed to linear form near its minima (see Fig. 2). If we define

\[ m = S' \cos \theta; \] (5.4)

then

\[ U^-(m) = -\gamma S'^2 \cos^2 \theta - \alpha S' \sin \theta. \] (5.5)

The minima are located at \( \theta = \theta_1, \pi - \theta_1 \), where

\[ \sin \theta_1 = \alpha / 2\gamma S'. \] (5.6)

It follows that if \( \alpha \) and \( \gamma \) remain fixed as \( S \to \infty \), the minima approach the points \( m = \pm S' \), which gives us a problem similar to that of the previous section. For novelty’s sake, let us therefore take \( \alpha \) and \( \gamma \) to scale so that \( \theta_1 \) remains fixed and not close to 0 as \( S \to \infty \). We shall see that our final answer for \( \Delta_0 \) will hold even when this condition is not satisfied.

For future use, let us define \( \theta_0 \) as the angle at which the classical expression for the energy (not \( U^-(m) \)) has a minimum. We have

\[ \sin \theta_0 = \alpha / 2\gamma S. \] (5.7)

Further,

\[ \sin \theta_1 = (1 - (1/2S) + \cdots) \sin \theta_0; \quad \cos \theta_1 = \cos \theta_0 + \sin^2 \theta_0 / 2S \cos \theta_0 + \cdots. \] (5.8)

With the above conditions on \( \theta_1 \), it is easy to find \( C_m \) near the potential minima. Let us define

\[ m_1 = S' \cos \theta_1. \] (5.9)

The conditions on \( \alpha \) and \( \gamma \) imply that \( S - m_1 = O(S) \). Since the wavefunction we seek is essentially that for the ground state of a harmonic oscillator, its spatial extent, \( \Delta m \), on the other hand, is of order \( S^{1/2} \). This can be seen by expanding the semiclassical Hamiltonian in powers of \( q \) and \( m - m_1 \). We have

\[ \mathcal{H}_{sc}(q, m) = w(m) + 2t(m) \cos q \approx -\gamma S'^2 (1 + \sin^2 \theta_1) + \gamma S'^2 \sin^2 \theta_1 q^2 + \gamma \cot^2 \theta_1 (m - m_1)^2 + \cdots. \] (5.10)

The leading neglected terms are, ignoring \( S' \) independent constants, of order \( S'(m - m_1)q^2 \equiv h_1, \ S'^2 q^4 \equiv h_2, \) and \( (m - m_1)^3 / S' \equiv h_3 \). It follows that the small oscillation frequency \( \omega_0 \) and the ground state energy \( E_0 \) (in the absence of tunneling, needless to say) are given by

\[ \omega_0 = 2\gamma S' \cos \theta_1, \] (5.11)

\[ E_0 = -\gamma S'^2 (1 + \sin^2 \theta_1) + \gamma S' \cos \theta_1. \] (5.12)
The wavefunction can be written down directly as for a harmonic oscillator with a continuous spatial coordinate,

\[ C_m = \left( \frac{\cos \theta_1}{\pi S' \sin^2 \theta_1} \right)^{1/4} \exp \left( -\frac{\cos \theta_1}{2S' \sin^2 \theta_1} (m - m_1)^2 \right), \] (5.13)

which is already normalized to unity inside the well.

What is the range of validity of Eq. (5.13)? This can be found by demanding that the terms ignored, \( h_1, h_2, \) and \( h_3 \), be much smaller than \( \omega_0/2 \), the value of the \( q^2 \) and \( (m - m_1)^2 \) terms in Eq. (5.10). Since the kinetic and potential energies are equal for a harmonic oscillator, we have \( q^2 \propto (m - m_1)^2/S' \) in the region of validity. Thus, \( h_1 = O(m - m_1)^3/S' = O(h_3) \), and \( h_2 = O(m - m_1)^4/S'^2 \ll h_1, h_3 \). Demanding that \( \omega_0/2 \gg h_1 \), we find that Eq. (5.13) is valid provided

\[ |m - m_1| \ll (S')^{2/3}. \] (5.14)

Note that this range keeps us clear of the end point \( m = S \).

The second step is to find \( C_m \) in the classically forbidden region, especially near the point \( m = 0 \) (if \( S \) is integral) or \( m = 1/2 \) (if \( S \) is half-integral). Since \( q(m) \) is imaginary, we define \( q(m) = i\kappa(m) \), (5.15)

with \( \kappa(m) > 0 \). Using the basic definition (2.5) with the energy (5.12), we obtain

\[ \cosh \kappa(m) = \frac{\sin^2 \theta + \sin^2 \theta_1}{2 \sin \theta \sin \theta_1} - \frac{\cos \theta_1}{2S' \sin \theta \sin \theta_1} + O(S')^{-2}. \] (5.16)

Writing

\[ \kappa(m) = \kappa_0(m) + \kappa_1(m) + \cdots, \] (5.17)

where \( \kappa_j \) is of order \( 1/S'^j \), we obtain

\[ \kappa_0(m) = \frac{1}{2} \log \left( \frac{S'^2 - m^2}{S'^2 \sin^2 \theta_1} \right), \] (5.18)

\[ \kappa_1(m) = \frac{1}{2} \left[ \frac{1}{m - m_1} - \frac{1}{m + m_1} \right]. \] (5.19)

The exponent in Eq. (2.7) therefore equals

\[ \phi(m) = \phi_0(m) + \phi_1(m) \]

\[ = \frac{1}{2} \left[ (S' + m) \log(S' + m) - (S' - m) \log(S' - m) - 2m \log(eS' \sin \theta_1) \right] \]

\[ + \frac{1}{2} \left[ \log(m_1 - m) - \log(m_1 + m) \right]. \] (5.20)

Here, \( \phi_0 \) and \( \phi_1 \) are the quantities given on the first and second lines above, and correspond, respectively, to \( \kappa_0 \) and \( \kappa_1 \).

The velocity is now easy to find. To leading order in \( S \), we get
\[ |v(m)| = 2\gamma S'^2 \sin \theta_1 \sin \theta \times \sinh \kappa_0 = \gamma (m_1^2 - m^2). \] (5.21)

The wavefunction in the central region therefore equals

\[ C_m = \frac{A}{m + m_1} \exp \phi_0(m), \] (5.22)

where \( A \) is a constant that must be found by matching the solution with Eq. (5.13). This in turn is done by expanding \( \phi_0(m) \) in powers of \( m - m_1 \), which is permissible as \( |m - m_1| \ll S'^{2/3} \) in the matching region. We find

\[ \phi_0(m) = \phi_{00} - \frac{\cos \theta_1}{2S' \sin^2 \theta_1} (m - m_1)^2; \] (5.23)

\[ \phi_{00} = S' [\log \cot(\theta_1/2) - \cos \theta_1]. \] (5.24)

Putting \( m = m_1 \) in the pre-exponential factor in Eq. (5.22), we see that the forbidden region \( C_m \) has exactly the structure required to match on to Eq. (5.13). Comparing the two expressions, we obtain

\[ A = 2m_1 \left( \frac{\cos \theta_1}{\pi S' \sin^2 \theta_1} \right)^{1/4} e^{-\phi_{00}}. \] (5.25)

The final step is to apply the formula (3.11) for the splitting. In doing this, the following simplifications are useful. First,

\[ \phi_0(m) = -m \log \sin \theta_1 \quad \text{for} \quad m = O(1). \] (5.26)

Second, to leading order in \( S \),

\[ \omega_0 = 2\gamma S \cos \theta_0. \] (5.27)

Collecting together all these facts, we obtain, for both integral and half-integral \( S \),

\[ \Delta_0 = 4\omega_0 \left( \frac{S}{\pi} \right)^{1/2} \frac{\cos^{3/2} \theta_0}{\sin \theta_0} \left( \frac{1 - \cos \theta_0}{1 + \cos \theta_0} \right)^{S + 1/2} e^{2S \cos \theta_0}. \] (5.28)

This is the main result of this section. It can be seen to be identical to Eq. (16) of Enz and Schilling [7], via the substitutions \( A = \gamma, a = \sin \theta_0 \) and \( b = 0+ \). It is almost, but not quite identical to Eq. (4.11) of Garg and Kim [12], which errs by a factor of \( O(S^0) \).

Several comments about Eq. (5.28) are in order. First, although we have only derived it assuming that \( \sin \theta_0 \gg 1/S \), it holds in fact for all \( \sin \theta_0 \), provided of course that the WKB approximation itself is valid. This can be seen from the numerical comparison we give below, and also analytically, by assuming that \( \sin \theta_0 = O(1/S) \) from the very start. This suggests that Eq. (5.28) holds uniformly for all \( \sin \theta_0 \) not too close to 1, but we have not investigated this point carefully. As a subcomment, note that in the limit \( \theta_0 \to 0 \), i.e., vanishing \( \alpha \), \( \Delta_0 \sim \alpha^{2S} \). This is of course, exactly what is expected from perturbation theory — it takes \( 2S \) applications of the perturbation \(-\alpha S_x\) to connect the states with \( S_z = \pm S \) [28]. Second, the WKB validity restriction means that the field \( \alpha \) in Eq. (1.13) can not be
too large. Quantitatively, we require that the energy barrier be much greater than $\omega_0$, the level spacing in the well. This condition can be shown to be equivalent to

$$1 - \sin \theta_0 \gg S^{-2/3}.$$  \hfill (5.29)

Third, as long as Eq. (5.29) holds, in the limit where the field is large and the barrier is small, Eq. (5.28) reduces to

$$\Delta_0 = 4\sqrt{3}\omega_0 (B_0/2\pi)^{1/2} e^{-B_0},$$  \hfill (5.30)

where $B_0 = (2/3)S \cos^3 \theta_0 = (16/3)\Delta U/\omega_0$, $\Delta U$ being the energy barrier. This form is the well known answer for the tunnel splitting of a massive particle moving in a quartic potential double well. The spin problem can be transformed into such a problem by noting that (i) in this limit $S_z \approx S$, so that the commutator $[S_y, S_z] = iS_x$ can be approximately reproduced by writing $S_z = x$, $S_y = -Sp$, where $p$ and $x$ are momentum and position operators with the commutator $[p, x] = -i$, and (ii) expanding the square root in the relation $S_x = \left[S^2 - (S_y^2 + S_z^2)\right]^{1/2}$, and rewriting $S_y$ and $S_z$ in terms of $p$ and $x$ as indicated above.

We leave it to the reader to check that the frequency $\omega_0$ and energy barrier $\Delta U$ of this particle problem are given by $2\gamma S \cos \theta_0$ and $\gamma S^2 \cos^3 \theta_0/4$, so that the answer for $\Delta_0$ is indeed given by Eq. (5.30).

Fourth, let us compare our result for $\Delta_0$ with the numerical and analytic answers obtained by van Hemmen and Sütő [19], which apply when $\sin \theta_0 = O(1/S)$. This comparison is shown in Table II. The parameters are $\gamma = \alpha = 1$, and the two approximate forms for the splitting are given by

$$\Delta_{\text{asymp}} = 2\gamma S \exp[-2S \log(\gamma S)],$$  \hfill (5.31)

$$\Delta_{\text{int}} = \frac{\omega_0}{2} \exp\left[-\int_{-m_i}^{m_i} \cosh^{-1} \left(\frac{-E_0 - \gamma m^2}{\alpha [S(S + 1) - m^2]^{3/2}}\right)\right].$$  \hfill (5.32)

In Eq. (5.32), $\pm m_i$ are the classical turning points, where $E_0 = w(m)$, and $E_0$ is the numerically obtained ground state energy. van Hemmen and Sütő describe $\Delta_{\text{asymp}}$ as an “asymptotic” result, and $\Delta_{\text{int}}$ as the “exact WKB” answer. As can be seen from the columns containing the ratios of the splittings given by these formulas to the numerically found splittings, neither result asymptotes to the correct answer. [Recall that two functions $f(x)$ and $g(x)$ are said to be asymptotically equal as $x \to x_0$, i.e., $f(x) \sim g(x)$, if $f(x)/g(x) \to 1$ as $x \to x_0$.] $\Delta_{\text{asymp}}$ actually gets worse with increasing $S$, which indicates that a multiplicative term such as $e^{-cS}$ has been omitted ($c$ is some constant), while $\Delta_{\text{int}}$ is off by a term of $S^0$ [29]. Neither result therefore meets the goal set in Sec. I of our paper: to find all terms $B_n$ in Eq. (1.3) that are of order $S^0$ or greater. Equation (5.23), on the other hand, does just that. It is also obvious that the recipe given by van Hemmen and Sütő [see Eq. (5.19) of Ref. [19]] cannot really be exact in general as regards the prefactor.

Lastly, Eq. (5.28) can be compared with the answer obtained by Scharf, Wreszinski, and van Hemmen [14], which is valid when $\sin \theta_0 = O(1/S)$. Their result — see their Eqs. (1.7) and (1.8), and Table 1 — is also off by $O(S^0)$. In fact the discrepancy is again $(e/\pi)^{1/2}$, which is to be expected in light of their method [29].
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Readers may wonder if all that is wrong with van Hemmen and Sütő’s formula is the typographical omission of a factor of $2^{-1/2}$. This is not so. An inspection of the arguments accompanying their Eqs. (5.19) and (C.10-12) reveals that there is no scope for such a factor and it is purely accidental that the error seems to be $2^{1/2}$ in this case. Indeed, use of a similar formula for potential problems with massive particles in one dimension also yields incorrect prefactors; for the quartic double well, e.g., the error is known to be $(e/\pi)^{1/2}$. The same error is present in Scharf, Wreszinski, and van Hemmen’s result [14].
FIGURES

FIG. 1. Discrete WKB potential energy diagram for tunnel splitting problem. For a particle with energy $E_0$, the region between $j_1$ and $j_2$ is classically forbidden.

FIG. 2. Sketch of the band-edge functions for the Hamiltonian (1.5). The key point is that $U^-(m)$ now has a quadratic minimum.
TABLES

TABLE I. Comparison between numerical and analytical [Eq. (4.31)] results for the ground state tunnel splitting for the Hamiltonian (1.1). Numbers in parentheses give the power of 10 multiplying the answer. We have chosen $k_1 = 5.0/S$, $k_2 = 20.0/S$. This scaling keeps $\omega_0$ fixed as $S \to \infty$.

| $S$ | $\Delta_0$ (numerical) | $\Delta_0$ (analytic) | Error(%) |
|-----|-----------------------|-----------------------|----------|
| 10  | 9.282(-3)             | 9.749(-3)             | 5.0      |
| 11  | 3.738(-3)             | 3.906(-3)             | 4.5      |
| 12  | 1.497(-3)             | 1.558(-3)             | 4.1      |
| 13  | 5.974(-4)             | 6.195(-4)             | 3.7      |
| 14  | 2.375(-4)             | 2.455(-4)             | 3.4      |
| 15  | 9.412(-5)             | 9.708(-5)             | 3.1      |
| 16  | 3.721(-5)             | 3.830(-5)             | 2.9      |
| 17  | 1.468(-5)             | 1.508(-5)             | 2.7      |
| 18  | 5.778(-6)             | 5.927(-6)             | 2.6      |
| 19  | 2.271(-6)             | 2.326(-6)             | 2.4      |
| 20  | 8.910(-7)             | 9.115(-7)             | 2.3      |

TABLE II. Comparison between numerical and various analytical and semianalytical results for the ground state tunnel splitting of the Hamiltonian (1.5). The parameters are $\alpha = \gamma = 1$. As in Table I, $x(n)$ denotes the number $x \times 10^n$. The quantities $\Delta_n$, $\Delta_{\text{asymp}}$, and $\Delta_{\text{int}}$ are taken from Table I of van Hemmen and Sütő[19], and are, respectively, the numerically computed splitting, the result (5.31), and the numerically evaluated integral expression (5.32). The quantity $\Delta_0$ is given by Eq. (5.28) of this work.

| $S$ | $\Delta_n$ | $\Delta_{\text{asymp}}$ | $\Delta_{\text{asymp}}/\Delta_n$ | $\Delta_{\text{int}}$ | $\Delta_{\text{int}}/\Delta_n$ | $\Delta_0$ | $\Delta_0/\Delta_n$ |
|-----|-------------|--------------------------|----------------------------------|-----------------------|---------------------------------|-------------|---------------------|
| 3   | 1.44(-3)    | 4.12(-3)                 | 2.86                             | 2.01(-3)              | 1.40                            | 1.48(-3)    | 1.03                |
| 4   | 1.18(-5)    | 6.10(-5)                 | 5.17                             | 1.64(-5)              | 1.39                            | 1.20(-5)    | 1.02                |
| 5   | 5.18(-8)    | 5.12(-7)                 | 9.88                             | 7.25(-8)              | 1.40                            | 5.24(-8)    | 1.01                |
| 6   | 1.43(-10)   | 2.76(-9)                 | 19.3                             | 2.00(-10)             | 1.40                            | 1.44(-10)   | 1.01                |
| 7   | 2.68(-13)   | 1.03(-11)                | 38.5                             | 3.77(-13)             | 1.41                            | 2.70(-13)   | 1.01                |
| 8   | 3.66(-16)   | 2.84(-14)                | 77.7                             | 5.15(-16)             | 1.41                            | 3.68(-16)   | 1.01                |
| 9   | 3.79(-19)   | 6.00(-17)                | 158                              | 5.36(-19)             | 1.41                            | 3.81(-19)   | 1.01                |
| 10  | 3.09(-22)   | 1.00(-19)                | 324                              | 4.37(-22)             | 1.41                            | 3.10(-22)   | 1.00                |
| 11  | 2.03(-25)   | 1.35(-22)                | 666                              | 2.87(-25)             | 1.41                            | 2.03(-25)   | 1.00                |

\(^{a}\)The numbers have been given to greater accuracy and corrected in a few places.
