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An Optimized Quadrature Scheme for Evaluating General Higher-Order Phase Integrals

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A quadrature scheme for evaluating general first- and higher-order phase integrals is presented that creates a more efficient, more stable, and more user-friendly computer code. By this means one can both gain the full power of the phase integral method and dispense with the use of JWKB results as initial guesses for "exact" numerical calculations. In such cases the high-order phase integral technique may ensure great accuracy with little computational cost and without any new fundamental modifications to the familiar JWKB procedure. The method is illustrated by determining complex Regge pole positions for a test potential.

1. INTRODUCTION

The higher-order phase integral method is a powerful tool for solving Sturm–Liouville systems [1]. The first-order version of the phase integral method, the JWKB-approximation, is used extensively because of its fundamental physical significance and computational cheapness. In the region of its validity, depending on the location of the turning points in the complex plane, the higher-order corrections of the phase integral method often ensure extreme speed combined with a precision not easily obtainable by any other method. In all cases, the higher-order terms have the fundamental role of providing a measure of the validity of the phase integral method, thus dispensing with comparison calculations with "exact" numerical methods—were results by such methods obtainable at all.

The applicability of the high-order forms of the phase integral method requires an effective technique for calculating the corresponding high-order phase integrals. In doing this, as described below, the main idea is the factorizing of the integrand into an analytical and a singular part. The former may then be accurately represented by polynomial series while the singular part is transformed to certain analytically handled, complex path integrals around the nonintegrable turning points. This technique, so far restricted to single well potentials, was first presented in [2, Method 2]. It yields some distinct advantages in practical calculations; the possibility of a code both flexible and weakly dependent on the potential and a straightforward generalization to a full complex formalism. This complex formalism

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phase integral method makes possible the extension of its range of applicability to various problems of scattering theory in which there are many very time-consuming problems. For instance, the partial wave representation of differential cross-section may need thousands of terms with accurate phase shifts and the need for an efficient computation procedure for them is obvious.

A preceding paper by our group presents methods for evaluating phase integrals in the most important cases of the distributions of the turning points [3]. Two techniques were devised for taking into account the numerical effects of the coalescence of an "internal" and an "external" turning point. Different quadrature intervals and mesh points for these Gaussian quadraturelike formulas were examined by explicitly inverting the corresponding Vandermonde matrices. The inexpediency of this approach lies in the numerical sensitivity of the inversion of high-order matrices. This obstacle was eliminated in [4] by adopting orthogonal basis polynomials to define the expansion coefficients. Paper [5] then presented the final generalization of this method to obtain first- and higher-order phase integrals for arbitrary complex turning points along implicitly defined complex contours. The effect of an "external" turning point was taken into account and the defining the quadrature intervals independent of the actual turning points was solved by choice of a suitable smoothing function. The extension of the quadrature interval is numerically effective in difficult high-order cases [3, 4]. Also, in subsequent computations with slightly different potential parameters, it may be expedient to utilize the same quadrature interval. However, this comprehensive procedure has two unsound features in extensive computations; the user needs some experience in choosing a suitable mesh number for the polynomial expansion, and the rapidly growing alternant combination coefficients make the calculation of the path integrals numerically unreliable.

The efficiency of the phase integral quadratures depends on the number of mesh points required to define the polynomial approximation. This varies considerably with the potential, with the order of approximation used, and, naturally, with the desired accuracy. Certainly, it is possible to implement a general code where all the practical considerations introduced in [5] are controlled by appropriate choices of different smoothing functions and quadrature intervals, but this may be accompanied by a loss of computational efficiency and comprehensibility of the program. Furthermore, when treating quadrature subroutines as "black boxes" it is of great importance to avoid accidental instabilities arising, for example, from an overly high accuracy requirement.

The purpose of the present article is to provide a computer code for handling practical problems, for users who lack a profound knowledge of the method. In the present version, the use of subroutines as "black boxes" is examined both when evaluating the smoothed (Sect. 3) and the singular (Sect. 4) integrand factors of the phase integrals. A new structure of mesh points has been chosen which automatically allows the use of a suitable mesh for each phase integral without a loss of computational economy. For the polynomial expansion, orthogonal Chebyshev polynomials are adopted, and with the aid of these fixed mesh points,

the real valued path integrals may be evaluated by direct recursion without resort to explicit polynomial expansion. A much more compact and efficient form of computation is achieved, which makes feasible more accurate, more extensive, or more complicated calculations. Although these advantages are gained at the cost of generality, this scheme of using fixed mesh points for separated turning points is capable of yielding accurate results in most realistic situations. It may be noted that the phase integral approximation becomes increasingly invalid when the coalescing of an "external" turning point leads to numerical difficulties, unless certain correction terms are included into the phase integrals [6, 7]. Such high-order correction functions are known for a very few cases, and there are excellent reasons for using the Prüfer phase function in combination with the phase integral approximation, when solving problems with coalescing turning points [1, 8].

In practical problems, for instance when determining quantum mechanical quantities by iterative procedures, the derivatives of various characteristic properties of the system, such as the energy, may be needed. In the phase integral approach, the problem is formulated as a function of the phase integrals via certain quantum conditions. Two advantages of this approach are the ease of formulating, for the phase integrals, the analytical derivatives with respect to these parameters, and the ease of implementing the problem numerically. In fact, the method to be described allows to code to yield automatically the desired energy derivatives of the phase integrals without an explicit definition in the user supplied nucleus. The computational cost of this gain is minimal, due to the similarity of the expressions for the quantum condition phase integrals and their derivatives.

In the following, the general description of the method is presented in Section 2. In Section 3, the numerical determination of the expansion coefficients by means of the new mesh points structure is illustrated, while the required weight integrals are evaluated in Section 4. The method is then illustrated by test calculations in Section 5.

2. Method

The phase integrals of interest may be written in the form

$$I_k(E) = \int_\Gamma dr\, f_k(r)/[E - U(r)]^{k+(1,2)}, \tag{1}$$

where $k \geqslant -1$ is an integer, $U(r)$ any smooth potential function, E the energy, and $f_k(r)$ some analytic combination of powers of r, $U(r)$ and its derivatives. Due to the integration path Γ in the complex r plane, there exist two types of phase integrals. The two-turning-points integrals are integrated along a loop Γ_{12} encircling the two turning points r_1, r_2, and the one-turning-point integrals are defined by a nonclosed path Γ_{b2} around the turning point r_2 with end points at different lips of the branch cut, as depicted in Fig. 1. At the turning points, defined as zeros of $[E - U(r)]$, the

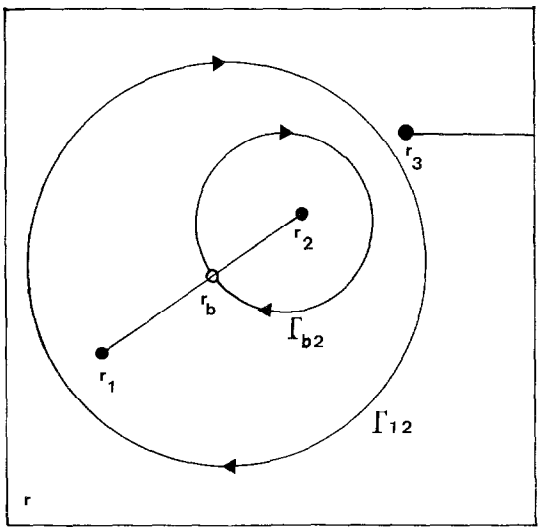

FIG. 1. Schematic drawing of the integration contours and of the distribution of turning points in the complex r plane. The points r_1 and r_2 are adjacent turning points defining a two-turning-points contour Γ_{12}. The point $r_b \in [r_1, r_2]$ is an integration point associated with a one-turning-point contour Γ_{b2}. r_3 denotes an external turning point outside the integration region.

high-order integrand $k > 0$ in Eq. (1), has nonintegrable singularities and in general E, $U(r)$, $f_k(r)$ and the turning points can take complex values. By the definition of the turning points, the factor $[E - U(r)]$ may be written as

$$E - U(r) = u(r) \prod_{\{r_i\}} (r_i - r), \tag{2}$$

where, assuming analytic $U(r)$ and simple zeros, $u(r)$ is analytic and different from zero at the turning points $\{r_i\}$ under consideration and in the region including no other turning points. In this region, $f_k(r)/[u(r)]^{k+(1/2)}$ is analytic and may be therein expanded to polynomial series.

For the two-turning-points integrals, a convenient expansion range for the analytical part of the integrand in Eq. (1) is $[r_1, r_2]$ between the turning points. The Chebyshev polynomials are used as basis functions and the orthogonal range $[-1, 1]$ is achieved by defining the change of variables

$$r = \tfrac{1}{2}(r_1 + r_2) + \tfrac{1}{2}(r_2 - r_1)\, z. \tag{3}$$

By introducing the notation ($\dot{r} = dr/dz$)

$$F(z) = f_k(r)/[Au(r)]^{k+(1/2)}\, \dot{r}, \tag{4}$$

where the dimensionless factor A depends on the number of turning points, the phase integral may be written in the form

$$I_k(E) = \int_{\Gamma'_{12}} dz\, F(z)/[1-z^2]^{k+(1/2)}, \tag{5}$$

where Γ'_{12} is the integration path around the points ± 1 in the z plane corresponding to Γ_{12} in the r plane. By approximating the analytical $F(z)$ as a truncated Chebyshev expansion

$$F(z) \simeq \sum_{n=0}^{N}{}' b_n T_n(z) \tag{6}$$

and by introducing the notation

$$\int_{\Gamma'_{12}} dz\, T_n(z)/[1-z^2]^{k+(1/2)} = J_2^T(k, n), \tag{7}$$

the phase integral takes the form

$$I_k(E) = \sum_{n=0}^{N}{}' b_n J_2^T(k, n) = \sum_{n=0}^{N,2}{}' b_{2n} J_2^T(k, 2n), \tag{8}$$

where, for later convenience, the notation $\sum'$ means a sum with the first term halved; $\sum'^{N}_{n=0} a_n = a_0/2 + a_1 + \cdots + a_N$. The summations can be taken over only even values of n because $J_2^T(k, n)$ vanishes for odd n (see Sect. 4).

In the case of one-turning-point integrals, the procedure is the same as above but a suitable expansion range is $[r_b, r_2]$ between the integration point r_b and the turning point, corresponding to Fig. 1. A convenient change of the variable is now

$$r = r_b + (r_2 - r_b)\, z \tag{9}$$

yielding for $F(z)$ in Eq. (4) the Chebyshev series representation

$$F(z) \simeq \sum_{n=0}^{N}{}' b_n T_n^*(z) \tag{10}$$

with basis polynomials $T_n^*(z)$ orthogonal on the range $[0, 1]$. In applications where the integration point r_b approaches infinity it is best to write out explicitly the contribution $F(z=0)$, which is determined by the boundary conditions, against the disadvantage of overflow. For one turning point the reference function to be used is $[1-z]$, corresponding to Eq. (5), and the definition of the required weight integral has the form

$$\int_{\Gamma'_{b2}} dz\, T_n^*(z)/[1-z]^{k+(1/2)} = J_1^{T^*}(k, n) \tag{11}$$

with Γ'_{b2} corresponding to Γ_{b2} yielding

$$I_k(E) = \sum_{n=0}^{N}{}' b_n J_1^{T*}(k, n). \tag{12}$$

Generally, one of the most important concepts used in numerical problems is the method of successive approximations. Among such techniques the Newton–Raphson-type iteration methods effectively utilize the derivatives of the iteration equation. For the phase integrals of Eq. (1), which are functions of certain potential parameters, the analytical derivatives are commonly easy to derive and in the region of validity of the phase integral method the phase integrals are typically smooth functions of these parameters. Thus the desired iteration procedure may be achieved without any doubt regarding the correct convergence restrictions or appropriate initial values and step sizes. Particularly, the form of the corresponding derivative with respect to energy is simply

$$\frac{\partial[I_k(E)]}{\partial E} = -\left(k+\frac{1}{2}\right) I_{k+1}(E); \tag{13}$$

and because $f_{k+1} = f_k$ in Eq. (1), the first and higher derivatives are extremely efficient to compute once $I_k(E)$ has been evaluated, since most of the computational work for $I_{k+1}(E)$ having already been performed in computing $I_k(E)$. Furthermore, the above means that in determining real or complex energy eigenvalues, the initial value of energy can not only be crude but even completely wrong, because in the phase integral formalism each eigenvalue is unambiguously associated with a quantum number, which is not always easy to implement for direct numerical techniques.

It may be noted that when the expansion coefficients b_n of $F(z)$ are numerically calculated, as will be described in Section 3, the turning points are not special points and the numerical work can be done without worry about the actual location of branch cuts caused by the multiply valued integrand in Eq. (1). This multiple valuedness is encountered in evaluating the weight integrals J_2^T or J_1^{T*}, but it is dealt with analytically, as will be described in Section 4, and the topologically proper integration paths are achieved by a direct definition.

3. Mesh Points

In the case of two turning points, the expansion coefficients of $F(z)$ in Eq. (6) are

$$b_n = \frac{2}{\pi}\int_{-1}^{1} dz\, F(z)\, T_n(z)/\sqrt{1-z^2} \tag{14}$$

and the actual task is the choice of the quadrature scheme and the quadrature points for the integral in Eq. (14). An obvious approach is the usual N-point

Gaussian quadrature, the zeroes of an Nth order orthogonal polynomial chosen for quadrature points. One choice is the zeros of the Chebyshev polynomial $T_N(z) = \cos[N \arccos(z)]$,

$$z_m'^{(N)} = \cos\left[\frac{(2m-1)}{2N}\pi\right], \qquad m = 1,..., N \tag{15}$$

to approximate the coefficients b_n [5]. Another possibility is, however, the use of the points at which $|T_N(z)| = 1$, the extrema of $T_N(z)$

$$z_m^{(N)} = \cos\left(\frac{m}{N}\pi\right), \qquad m = 0,..., N \tag{16}$$

yielding the approximation for expansion coefficients [9]

$$b_n \simeq b_n^{(N)} = \frac{2}{N}\sum_{m=0}^{N}{}'' F(z_m^{(N)})\, T_n(z_m^{(N)}), \qquad n = 0,..., N-1, \tag{17}$$

where $\sum''$ is a "trapezoidal" sum, i.e., $\sum''_{n=0}^{N} a_n = a_0/2 + a_1 + \cdots + a_{n-1} + a_N/2$. Equation (17) holds for $n = N$ with the correspondence $b_N \simeq \frac{1}{2} b_N^{(N)}$. The expression in Eq. (17) is exact for a polynomial $F(z)\, T_n(z)$ of order up to $2N-1$, due to the discrete orthogonality of Chebyshev polynomials at the extrema ($n, n' \leqslant N$)

$$\sum_{m=0}^{N}{}'' T_n(z_m^{(N)})\, T_{n'}(z_m^{(N)}) = \begin{cases} 0, & n \neq n' \\ N/2, & n = n' \neq 0, N \\ N, & n = n' = 0, N. \end{cases} \tag{18}$$

The use of the extrema offers some computational advantages. The doubling of the number of mesh points to $2N$ makes only N new mesh points necessary because

$$\{z_m^{(2N)}\}_0^{2N} = \{z_m^{(N)}\}_0^{N} \cup \{z_m'^{(N)}\}_1^{N} \tag{19}$$

with the fixed points $\{-1, 0, 1\} = \{z_m^{(2)}\}_0^2$, allowing an adaptive program code with minimum function evaluations. Corresponding to Eq. (19), the expansion coefficients with doubled mesh may now be written recursively by summing separately over the odd and the even values of m,

$$\begin{aligned} b_n^{(2N)} &= \frac{2}{2N}\sum_{m=0}^{2N}{}'' F(z_m^{(2N)})\, T_n(z_m^{(2N)}) \\ &= \frac{1}{2}\left[\frac{2}{N}\sum_{m=0}^{N}{}'' F(z_m^{(N)})\, T_n(z_m^{(N)}) + \frac{2}{N}\sum_{m=1}^{N} F(z_m'^{(N)})\, T_n(z_m'^{(N)})\right] \\ &= \frac{1}{2}(b_n^{(N)} + b_n'^{(N)}), \qquad n = 0,..., N-1, \end{aligned} \tag{20}$$

where the last sum over m, $b_n'^{(N)}$, is just the N zero points quadrature form for b_n [5]. The $N+1$ last coefficients are directly formed by

$$b_{2N-n}^{(2N)} = \tfrac{1}{2}(b_n^{(N)} - b_n'^{(N)}), \qquad n = 0,..., N \tag{21}$$

if only the $b_n'^{(N)}$ are computed for n values up to $N-1$ ($b_N'^{(N)} = 0$), because of the symmetry properties of $T_n(z)$ at the extreme

$$(-1)^m T_{2N-n}(z_m^{(2N)}) = T_n(z_m^{(2N)}) = T_m(z_n^{(2N)}), \qquad n = 0,..., N. \tag{22}$$

Corresponding to the two last equations, it is possible to minimize storage requirement, if desired, for example for microcomputer adaptations. The particular simple form of the coefficient $b_N^{(N)} = (2/N) \sum''_{m=0}{}^{N} (-1)^m F(z_m^{(N)})$ is remarkable. In practical calculations of the phase integral $I_k(E)$ it is convenient to double the number of mesh points N until either the absolute value of the term $b_N^{(N)} J_2^T(k, N)$, according to Eq. (8), has reached some prescribed accuracy requirement, or $b_N^{(N)}$ has converged to the relative machine accuracy parameter. Once the $b_n^{(N)}$ have converged with a suitable accuracy to the expansion coefficients b_n, in summing over n in Eq. (8), the last calculated term may be used as a truncation option.

In the case of the one-turning-point procedure, the expansion coefficients are achieved as in Eq. (17) by determining formally $F(z) = F^*(z^*) = F^*[(\frac{1}{2}(z+1)]$, because $T_n^*(z^*) = T_n(z)$ by the definition of Chebyshev polynomials orthogonal on the range $[0, 1]$. In this case the b_n for odd values of n are also required.

As a final practical point it is to be noted that $F(z)$ in Eq. (4) is not well defined at the turning points ± 1 in the z plane when the poles of $1/[E - U(r)]$ are removed by direct multiplication by the reference function $(1-z^2)$ or $(1-z)$. At these points $F(z)$ can still be easily calculated by using l'Hospital's rule for the required expressions as follows ($\dot{r} = dr/dz$), $\lim_{z \to \pm 1} [1-z^2]/[E-U(r)] = \pm 2/[U'(r)\,\dot{r}]\,|_{r=r(\pm 1)}$ or $\lim_{r \to 1} [1-z]/[E-U(r)] = 1/[U'(r)\,\dot{r}]\,|_{r=r(1)}$, the prime denoting derivation with respect to r. These evaluations at the turning points are required only once for each phase integral, while for higher-order integrals the routines for the derivatives of $U(r)$ are needed in any case.

4. Weight Integrals

The weight integrals to be evaluated are $J_2^T(k, n)$ in the case of the two-turning-points phase integrals and $J_1^{T^*}(k, n)$ for the one-turning-point integrals,

$$J_2^T(k, n) = \int_{\Gamma_{12}} dz\, T_n(z)/[1-z^2]^{k+(1/2)}, \tag{23}$$

$$J_1^{T^*}(k, n) = \int_{\Gamma_{b2}} dz\, T_n^*(z)/[1-z]^{k+(1/2)}. \tag{24}$$

These integrals are well defined by their integration paths Γ'_{12} and Γ'_{b2} in the z plane which is mapped from the r plane by linear transformations defined by transforming either the range $[r_1, r_2]$ onto $[-1, 1]$ or the range $[r_b, r_2]$ onto $[0, 1]$, respectively. As depicted in Fig. 1, the proper integration paths are defined as paths encircling the turning points under consideration and not crossing the branch cuts emerging from the turning points and without concern for a numerical determination of the course of the paths. In addition, all the integrals $J_2^T(k, n)$ and $J_1^{T^*}(k, n)$ will be real.

In the earlier version of the quadrature procedure [5], the weight integrals $J_2^T(k, n)$ and $J_1^{T^*}(k, n)$ were evaluated with the help of recursion relations of the simpler weight integrals, where in Eqs. (23) and (24) the basis functions $T_n(z)$ or $T_n^*(z)$ have been replaced with the basis $\{z^n\}$, by forming a linear combination of these simpler weight integrals through the use of the coefficients of Chebyshev polynomials as combination coefficients. This method, however, although exact in principle, is a numerically badly conceived calculation because of the rapidly growing alternant sign coefficients, which may cause numerical instability even at moderate values of n. This instability may be avoided by using the general recursion properties of the orthogonal polynomials yielding directly a much more compact and computationally favorable recursion form for the weight integrals $J_2^T(k, n)$ and $J_1^{T^*}(k, n)$.

In the case of the two-turning-points integrals, the basic steps are the recursion properties of $T_n(z)$ as follows

$$T_{n+2}(z) = 2zT_{n+1}(z) - T_n(z), \qquad n \geqslant 0, \tag{25}$$

$$T'_{n+1}(z) = 2(n+1)\, T_n(z) + \frac{n+1}{n-1}\, T'_{n-1}(z), \qquad n \geqslant 2 \tag{26}$$

the prime denoting derivatives with respect to z. The integrand resulting from the first term of the right side of Eq. (25) may be evaluated by integration by parts yielding

$$\int_{\Gamma'_{12}} dz\, 2zT_{n+1}(z)/[1-z^2]^{k+(1/2)} = \frac{2}{1-2k} \int_{\Gamma'_{12}} dz\, T'_{n+1}(z)/[1-z^2]^{k-(1/2)}$$

$$= \frac{4(n+1)}{1-2k} \sum_{m=0}^{n}{}' \int_{\Gamma'_{12}} dz\, T_m(z)/[1-z^2]^{k-(1/2)}, \qquad n \geqslant 2 \tag{27}$$

the prime denoting a halved term in summing with $m = 0$, where the last expansion is obtained by substituting $n/2$ times Eq. (26) and by observing that $T'_1(z) = T_0(z)$. Here, only even values of n and m may be assumed because the parity of $T_n(z)$ behaves as n and on the loop Γ'_{12} all $J_2^T(k, n)$ vanish for n odd. In addition, the first nonzero value of $J_2^T(k, n)$ exists when $n = 2k > 0$, taking the value $-(-1)^k 2^{2k}\pi$, where 2^{2k-1} is the leading coefficient of the polynomial $T_{2k}(z)$, which may be obtained by expanding the factor $[1-z^2]^{-k-(1/2)}$ as a binomial series on the circle

centered at $z=0$ with a radius greater than unity. Thus the recursion formula with respect to n and k is

$$J_2^T(k, n+2) = -J_2^T(k, n) + \frac{4(n+1)}{1-2k} \sum_{m=k-1}^{n/2,} J_2^T(k-1, 2m), \tag{28}$$

when $n/2 \geqslant k-1 \geqslant 0$. For the initial value $k=0$, the turning points $z=\pm 1$ are integrable singularities yielding $J_2^T(0, 0) = -2\pi$ and the vanishing of all $J_2^T(0, n)$ when $n \neq 0$ because of the orthogonality of Chebyshev polynomials and because $T_0(z)=1$, corresponding to Eq. (14). For this reason, the recursion relation in Eq. (28) is considerably simplified for $k=1$, yielding simply $J_2^T(1, n) = n2\pi$ for even $n \geqslant 2$. Corresponding to this simplicity, the third-order terms ($k=1$) in phase integral calculations may now be implemented for restricted problems even with an ordinary programmable pocket calculator, a point which may be of practical significance, because in the region of validity of the method the accuracy ensured by the third-order correction is sufficient for most practical applications. This point will shortly be discussed by a sample calculation in Section 5.

In the case of the one-turning-point integrals, the desired recursion formula may be introduced by recurring to the polynomials $T_n(z)$ orthogonal on the usual range $[-1, 1]$ with the help of the relations

$$T_n^*(z) = (-1)^n T_n^*(1-z) = T_{2n}(\sqrt{z}). \tag{29}$$

Corresponding to the last equation, the change of variable $q = \sqrt{1-z}$ is introduced, in which case the integration path Γ'_{b2} is deformed to the path from -1 to 1 avoiding the singular point $q=0$. The weight integral may now be written in the form

$$\int_{\Gamma'_{bz}} dz\, T_n^*(z)/[1-z]^{k+(1/2)} = -2(-1)^n \int_{-1}^{1} dq\, T_{2n}(q)/q^{2k}. \tag{30}$$

According to Eq. (25)

$$\int_{-1}^{1} dq\, T_{2n+2}(q)/q^{2k} = 2\int_{-1}^{1} dq\, T_{2n+1}(q)/q^{2k-1} - \int_{-1}^{1} dq\, T_{2n}(q)/q^{2k} \tag{31}$$

and after $n+1 \geqslant 1$ substitutions as above, the final recursion will have the form

$$J_1^{T*}(k, n+1) = -J_1^{T*}(k, n) + 4 \sum_{m=0}^{n}{}' (-1)^{n-m} J_1^{T*}(k-1, m) \tag{32}$$

the prime denoting a halved first term in the cumulative sum over m. The required weight integrals with initial value $k=0$ are easily evaluated with the aid of Eq. (26) when

$$J_1^{T*}(0, n) = -2(-1)^n \int_{-1}^{1} dq\, T_{2n}(q) = \frac{(-1)^n 4}{4n^2-1}, \tag{33}$$

because $T_n(\pm 1) = (\pm 1)^n$. As a final step, the required weight integrals with the initial value $n = 0$ are obtained by a direct integration

$$J_1^{T*}(k, 0) = -2 \int_{-1}^{1} dq/q^{2k} = -\frac{4}{1-2k}. \tag{34}$$

Note that although the first order phase integrals have $k = -1$ in Eq. (1), the singularities at the points $z = \pm 1$ may still be removed by multiplication with $[1-z^2]$ or $[1-z]$; the initial value $k = 0$ in the recursion for the corresponding weight integrals may thus be used. Actually, in the case of the two-turning-points calculations, the evaluation of the phase integral in Eq. (8) is reduced to the familiar Gauss–Chebyshev quadrature at the extrema, when $k = -1$ or 0 in Eq. (1), because the only nonvanishing $J_2^T(0, n)$ has $n = 0$, and the absolute value of b_N may be used as the measure of the accuracy of the quadrature.

5. Numerical Tests

In order to test the method described above, the higher-order Regge pole positions up to fifth-order were computed. The effective potential $U(r)$ is defined by

$$U(r) = V(r) + l(l+1)/\beta^2/r^2, \tag{35}$$

where $\beta^2 = 2\mu/\hbar^2$ and

$$V(r) = \varepsilon \left[\left(\frac{r_m}{r} \right)^{12} - 2 \left(\frac{r_m}{r} \right)^{6} \right] \tag{36}$$

is a LJ(12, 6) potential with the parameters $\varepsilon = 4.0 \times 10^{-21}$ J, $r_m = 4.0 \times 10^{-10}$ m, and $\mu = 4.377 \times 10^{-26}$ kg, corresponding approximately to the elastic scattering of K by HBr [10]. The real energy parameter $E = 2.0 \times 10^{-20}$ J was used and in Regge-pole theory the orbital angular momentum number $l = l_n$ is allowed to take on complex values [11]. The calculations were carried with the value of the Planck constant $\hbar = 1.0543 \times 10^{-34}$ J. The expressions for $f_k(r)$ in Eq. (1) in the case of third- ($k = 1$) and fifth-order ($k = 3$) corrections are given in [5] and the six-decimal Regge pole positions l_n for $n = 0, 1, \ldots, 9$ and $n = 10, 20, \ldots, 100$ are presented in Table I. The quantal results have been calculated to three decimal places which differ in their last digit from those given here, corresponding to the accuracy of the parameters given in [12]. The values in Table 3 of [12] may be obtained by using in phase integral calculations the value of the Planck constant $\hbar = 1.054345 \times 10^{-34}$ J. An analysis of the higher-order contributions to the pole positions of Table I indicates that the third-order values are accurate to six, seven, or eight decimal places for both real and imaginary parts of pole positions l_n, $n = 0$, $n = 50$, or $n = 100$, respectively, and that the accuracy of the fifth-order results is even better whereas the first-order calculations yielded two-decimal accuracy for all the pole positions above. For all

TABLE I

Regge Pole Positions l_n for $n = 0, 1, ..., 9$ and $n = 10, 20, ..., 100$

n	Re l_n	Im l_n	n	Re l_n	Im l_n
0	180.018697	21.219655	10	175.080666	50.561778
1	179.245735	24.035487	20	176.193680	79.645373
2	178.529636	26.890830	30	181.148497	105.787244
3	177.873313	29.780920	40	187.632608	128.786442
4	177.279117	32.700804	50	194.432936	149.370767
5	176.748840	35.645416	60	201.103034	168.242410
6	176.283716	38.609632	70	207.522922	185.880999
7	175.884428	41.588342	80	213.682142	202.592714
8	175.551134	44.576508	90	219.601053	218.576896
9	175.283485	47.569226	100	225.305716	233.969174

pole positions l_n, $n = 0, ..., 100$, the simple Bohr–Sommerfeld quantization formula was used [12] because of the well-separated distribution of the turning points, allowing a very simple iteration procedure such as using the previously iterated value of the pole position as an initial guess for the next pole. With these (wrong) initial guesses the iteration of the first hundred pole positions to six correct decimal places took about 0.15 sec CPU time/pole on a VAX11/750 computer.

The third-order two-turning-points phase integrals with accuracy requirement 1.0×10^{-6} need 7 ($n = 0$), 15 ($n = 50$), and 25 ($n = 100$) mesh points for polynomial approximation, the increase of mesh points for pole positions l_n with higher n values corresponding to the increase in the range of approximation $[r_1, r_2]$. In practice, no estimate of the number of mesh points is required because in the computation procedure the number of mesh points is automatically increased until either the desired or the highest possible accuracy is achieved.

Because the integrand in Eq. (1) is integrable in the region including no turning points, it may sometimes be more efficient to integrate the middle part $[r_a, r_b] \subset [r_1, r_2]$ sufficiently far from the turning points by some standard integrator and to evaluate separately both contributions near the turning points by a one-turning-point procedure. Such cases may occur when the turning points are far apart or when extremely high accuracy is required. For comparison with the previous method, the calculations were repeated by using the earlier version of the one-turning-point procedure [5]; when very high accuracy was required, for some pole positions, the calculation completely blew up because of the numerical sensitivity of that method. It is evident that in extensive calculations the accidental instability of this kind, which is avoided in the present method, may cause much confusion and wasted computation.

Another test case here is the determination of the energy eigenvalues of the Sturm–Liouville problem when $U(r) = r^4$ in Eq. (1). This problem is a well-known example of the breakdown of the JKWB-approximation when the energy tends to zero, which is not surprising, because of the coalescence of all four turning points of

the problem. On the other hand, for higher quantum numbers sufficient accuracy is achieved with higher-order phase integral calculations as discussed in [1], but the basic point here is to show that a problem like this can be solved even with an ordinary programmable calculator with program capacity of about 200 key instructions. For instance, by a third-order calculation of the eigenvalue E_{10} six-digit accuracy, $E_{10} = 50.2653$, was obtained.

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