PHYSICAL REVIEW A VOLUME 51, NUMBER 6 JUNE 1995

Dependence of the rate of convergence of the Rayleigh-Ritz method on a nonlinear parameter

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(Received 26 September 1994)

Numerical computation of optimum values for nonlinear parameters in a Rayleigh-Ritz variational trial function is considerably more difficult than numerical computation of optimum values for linear parameters. Thus, an analytic understanding of the mechanisms that determine these optimum values can be quite useful. Uniform asymptotic expansions can be used to explore these mechanisms for the nonlinear parameter that sets the length scale for a basis set. These uniform asymptotic expansions usually involve two or more different kinds of terms whose relative importance changes as the nonlinear parameter changes, with two different terms being equally important at the point where the nonlinear parameter has its optimum value. Interference effects between these different terms are typical, and tend to become most pronounced near the optimum value. These different kinds of terms arise from singularities of the wave function, from the neighborhood of the classical turning point for the basis functions, and/or from saddle points. Comparisons of theory with (numerical) experiment will be given for Rayleigh-Ritz calculations on three model problems that illustrate the kinds of terms listed above.

PACS number(s): 03.65.Ge, 31.15.Ar, 31.15.Pf, 02.70.−c

I. INTRODUCTION

The Rayleigh-Ritz variational method is widely used for calculating bound state energies and wave functions. The effectiveness of the method depends on the choice of basis functions. A well chosen basis will yield both rapid convergence and tractable matrix element integrals. It follows that an understanding of the factors that influence the convergence behavior is an important part of the practitioner's toolkit.

The art of fitting simple analytic functions to the empirically observed convergence behavior of Rayleigh-Ritz calculations has been practiced for a long time. A theory of rates of convergence that could be used to validate this curve fitting — and to warn of its pitfalls — was slow in coming. The most important early papers, by Kato [1], Schwartz [2], Lakin [3], and Klahn and Morgan [4], are discussed by Hill [5]. A readable introduction to these ideas can be found in the work of Morgan [6]. Rates of convergence of the partial-wave expansions of atomic correlation energies have been discussed by Kutzelnigg and Morgan [7]. The convergence behavior of Gaussian basis sets has been discussed in papers by Klopper and Kutzelnigg [8] and Kutzelnigg [9,10].

A typical Rayleigh-Ritz calculation uses a trial function that depends on a number of parameters. Optimum values for the parameters that enter linearly can be obtained by solving a matrix eigenvalue problem. Optimum values of nonlinear parameters have to be obtained via numerical minimization, which is much more expensive. It can also be difficult because the numerical algorithms used for the purpose can miss the global minimum and get trapped in local minima. Analytic formulas that give approximations to the optimum values of nonlinear parameters can save this expense; analytic insight into the minimization can help to locate the global minimum even if the task of minimization must be completed numerically. Analytic results of this kind require asymptotic expansions that are uniformly valid in the nonlinear parameter. Such expansions are more difficult to construct than (nonuniform) expansions of the type used in a previous paper by the present author on rates of convergence for the Rayleigh-Ritz variational method [5].

The notion of uniformity as it applies to asymptotic expansions can be understood by considering as an example the expansion coefficients $c_k(\alpha) = \langle \xi_k^{(\alpha)} | \psi \rangle$, which appear when a wave function $|\psi\rangle$ is expanded in a set of orthonormal basis vectors $|\xi_k^{(\alpha)}\rangle$ that depend on a parameter α, which could be the parameter that sets the length scale for the basis set. Roughly speaking, a large k asymptotic expansion of $c_k(\alpha)$ is uniformly valid in a parameter α for α in some domain $\mathcal{D}$ if the error of the approximation obtained by truncating the series can be made smaller than some prescribed error tolerance by making k sufficiently large, with the same sufficiently large k being adequate for all α in $\mathcal{D}$. In the present paper, α will be the parameter that sets the length scale for the basis set and the domain $\mathcal{D}$ will have to be large enough to include the optimum value of α. The notion of uniformity can be made precise by writing the asymptotic expansion in the form

$$c_k(\alpha) = \sum_{n=0}^{N} c_k^{(n)}(\alpha) + \varepsilon(N, \alpha) . \tag{1.1}$$

The terms $c_k^{(n)}(\alpha)$ and the error $\varepsilon(N, \alpha)$ are required to have the properties

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$$|c_k^{(n+1)}(\alpha)/c_k^{(n)}(\alpha)| \le \delta_k^{(n)}(\alpha), \tag{1.2}$$

$$|\varepsilon(N,\alpha)/c_k^{(N)}(\alpha)| \le \delta_k^{(\varepsilon,N)}(\alpha), \tag{1.3}$$

$$\lim_{k\to\infty} \delta_k^{(n)}(\alpha) = 0, \tag{1.4}$$

$$\lim_{k\to\infty} \delta_k^{(\varepsilon,N)}(\alpha) = 0. \tag{1.5}$$

Formulas (1.2) and (1.4) say that each term of the expansion (1.1) is much smaller than the preceding term if k is sufficiently large. Formulas (1.3) and (1.5) say that the error $\varepsilon(N,\alpha)$ is much smaller than the last term kept if k is sufficiently large. The asymptotic expansion (1.1) is said to be uniformly valid in α for α in some domain $\mathcal{D}$ if error bounds $\delta_k^{(n)}(\alpha)$ and $\delta_k^{(\varepsilon,N)}(\alpha)$ can be found that are independent of α and satisfy (1.4) and (1.5) for all α in $\mathcal{D}$.

The present paper is the first step in an effort to gain an analytic understanding of the minimization with respect to nonlinear parameters. It extends and improves on the methods developed in [5] for analyzing rates of convergence for the Rayleigh-Ritz method. The analytic mechanisms that determine the optimum value of the nonlinear parameter that sets the length scale for a basis set are the principal focus. These mechanisms are explored by choosing a basis $e_k(\alpha;z)$ of harmonic oscillator functions, defined by

$$e_k(\alpha;z) = \pi^{-1/4}2^{-k/2}(k!)^{-1/2} \times\alpha^{1/2}H_k(\alpha z)\exp\left(-\alpha^2z^2/2\right), \tag{1.6}$$

whose length scale is set by the nonlinear parameter α. The H_k in (1.6) are Hermite polynomials in standard notation (see [11], pp. 192–196, or [12], pp. 249–255). Variational trial functions of the form

$$\tilde{\psi}^{(\mathrm{RR};K)}(x) = \sum_{k=0}^{K} c_k e_k(\alpha;x) \tag{1.7}$$

are used to construct Rayleigh-Ritz variational approximations $E^{(\mathrm{RR};K)}(\alpha)$ to the exact ground state energies E of the Hamiltonians

$$H^{(a)} = -\frac{1}{2}\frac{d^2}{dx^2} - \frac{1}{\cosh^2(x)},\quad x\in(-\infty,\infty), \tag{1.8}$$

$$H^{(b)} = -\frac{1}{2}\frac{d^2}{dx^2} - \frac{1}{x},\quad x\in[0,\infty), \tag{1.9}$$

and

$$H^{(c)} = -\frac{d^2}{dx^2} + x^2 + \lambda x^4,\quad x\in(-\infty,\infty). \tag{1.10}$$

The Schrödinger equation for the Hamiltonian $H^{(a)}$ with its $\cosh^{-2}$ potential is an exactly solvable potential well model. The Hamiltonian $H^{(b)}$ is the Hamiltonian for the S states of the hydrogen atom when a factor of x from the volume element is included in the wave function. The Hamiltonian $H^{(c)}$ describes the anharmonic oscillator.

Uniform asymptotic expansions are used to calculate analytic approximations to the error $E^{(\mathrm{RR};K)}(\alpha) - E$ that are uniformly valid in α for K large; these analytic approximations to $E^{(\mathrm{RR};K)}(\alpha) - E$ are then minimized with respect to α to obtain analytic approximations to the optimum value of α as a function of K. These analytic approximations are compared with optimum values of α determined by purely numerical methods. The analytic approximations to optimum α are found to agree with the numerical optimization to several digits even for moderate values of K. The functional forms that follow from the theory tend to be more complicated than the simple forms usually used to fit empirically observed convergence behavior.

The three Hamiltonians (1.8)–(1.10) have been chosen to illustrate several different kinds of terms that can contribute to the large K asymptotic behavior of the error $E^{(\mathrm{RR};K)}(\alpha) - E$. For (1.8), the optimum value of α is determined by a competition between contributions from singularities of the wave function in the complex plane and contributions from the neighborhood of the classical turning points of the basis functions (1.6). The situation for (1.9) is similar, except that the singularities of the wave function in the complex plane are replaced by a singularity on the real axis. The situation for (1.10) is rather different, because the wave function for (1.10) has no singularities in the finite complex plane; in this case the contributions to the asymptotic behavior of the error come from a set of four saddle points in the complex plane that can move to the real axis, coalesce, and then move apart again as α increases. Although the calculations have all been performed for the basis functions (1.6), the author believes that the extension of the results to basis sets built from other classical orthogonal polynomials should be straightforward.

The paper is organized as follows. The extended and improved theory of rates of convergence for the Rayleigh-Ritz method is outlined in Sec. II. Section III summarizes needed properties of the basis functions (1.6). Sections IV, V, and VI discuss the Hamiltonians (1.8), (1.9), and (1.10), respectively. Section VII indicates how similar calculations can be carried out for basis sets built from other classical orthogonal polynomials. A number of computational details have been relegated to the Appendixes.

II. CONVERGENCE RATES FOR THE RAYLEIGH-RITZ VARIATIONAL METHOD

This section will outline a method for analyzing convergence rates for the Rayleigh-Ritz variational method, which extends and improves the method developed in [5]. The method as presented here is valid for both ground and excited states and can be used to calculate as many terms as may be needed in the asymptotic expansion of the error. The section begins by outlining the Rayleigh-Ritz approximation. Best approximation in a Hilbert space is discussed next. The rate of convergence for the Rayleigh-Ritz approximation is then obtained by establishing the connection between the Rayleigh-Ritz approximation and best approximation in a Hilbert space.

The Rayleigh-Ritz method looks for an approximation

$|\tilde{\psi}^{(\mathrm{RR};K)}\rangle$ to the exact wave function $|\psi\rangle$ of the form

$$|\tilde{\psi}^{(\mathrm{RR};K)}\rangle = \sum_{k=0}^{K} \tilde{c}_k^{(\mathrm{RR};K)} |\xi_k\rangle, \tag{2.1}$$

where the $|\xi_k\rangle$ are a set of linearly independent basis vectors that are complete in a function space that contains the desired exact wave function $|\psi\rangle$. It will be convenient to assume that the $|\xi_k\rangle$ are orthonormal in the Hilbert space L^2 of square integrable functions, so that

$$\langle \xi_k | \xi_\ell \rangle = \delta_{k,\ell}. \tag{2.2}$$

The coefficients $\tilde{c}_k^{(\mathrm{RR};K)}$ in the approximation (2.1), and the approximate energy eigenvalues $\tilde{E}^{(\mathrm{RR};K)}$ of a Hamiltonian H, are obtained by solving the matrix eigenvalue problem

$$\sum_{\ell=0}^{K} \langle | \xi_k | H | \xi_\ell \rangle \tilde{c}_\ell^{(\mathrm{RR};K)} = \tilde{E}^{(\mathrm{RR};K)} \tilde{c}_k^{(\mathrm{RR};K)}, \tag{2.3}$$

which is obtained by looking for the stationary values of the Rayleigh quotient

$$\langle \tilde{\psi}^{(\mathrm{RR};K)} | H | \tilde{\psi}^{(\mathrm{RR};K)} \rangle / \langle \tilde{\psi}^{(\mathrm{RR};K)} | \tilde{\psi}^{(\mathrm{RR};K)} \rangle \tag{2.4}$$

with respect to the coefficients $\tilde{c}_k^{(\mathrm{RR};K)}$. If the eigenvalues E_k of H for $0 \le k \le J$ are ordered so that $E_k \le E_{k+1}$, and if the eigenvalues $\tilde{E}_k^{(\mathrm{RR};K)}$ of the matrix eigenvalue problem (2.3) are ordered so that $\tilde{E}_k^{(\mathrm{RR};K)} \le \tilde{E}_{k+1}^{(\mathrm{RR};K)}$ for $0 \le k \le K$, then the eigenvalues of (2.3) are upper bounds to the eigenvalues of H: $E_k \le \tilde{E}_k^{(\mathrm{RR};K)}$ for $0 \le k \le \min(J, K)$. Physicists and chemists usually cite Hylleraas and Undheim [13] and MacDonald [14] for this result, which actually goes back to an 1890 paper of Poincaré, and was probably known to Lord Rayleigh. Proofs plus a brief history may be found in the first two chapters of Weinstein and Stenger [15].

A principal difficulty in the analysis of rates of convergence for the Rayleigh-Ritz method is the fact that the coefficient $\tilde{c}_k^{(\mathrm{RR};K)}$ of $|\xi_k\rangle$ in the approximation (2.1) changes as K is increased. A way around this difficulty uses an approximation $|\psi\rangle \approx |\tilde{\psi}^{(B;K)}\rangle$, given by

$$|\tilde{\psi}^{(B;K)}\rangle = \sum_{k=0}^{K} \hat{c}_k |\eta_k\rangle, \tag{2.5}$$

for which the coefficients $\hat{c}_k$ are independent of K, as an initial approximation (which is corrected later) to the approximation (2.1). The basis functions $|\eta_k\rangle$ in (2.5) are linear combinations of the basis functions $|\xi_k\rangle$ in (2.1):

$$|\xi_\ell\rangle = \sum_{k=0}^{\ell} U_{k,\ell} |\eta_k\rangle, \tag{2.6}$$

$$|\eta_\ell\rangle = \sum_{k=0}^{\ell} \left(U^{-1}\right)_{k,\ell} |\xi_k\rangle. \tag{2.7}$$

It is convenient to incorporate the summation limits in (2.6) and (2.7) in the coefficients and define $U_{k,\ell}$ and $\left(U^{-1}\right)_{k,\ell}$ to be upper triangular matrices:

$$U_{k,\ell} = \left(U^{-1}\right)_{k,\ell} = 0 \text{ for } k > \ell. \tag{2.8}$$

The basis vectors $|\eta_k\rangle$ are determined by the requirement that they be orthonormal in a Hilbert space whose inner product is obtained from a suitably chosen self-adjoint positive definite linear operator B. If $|\mu\rangle$ and $|\nu\rangle$ are vectors in a linear space S, the quadratic form $\langle \mu | B | \nu \rangle$ associated with B satisfies all of the axioms for an inner product and can be used to construct the norm

$$\| \, |\nu\rangle \, \|_B = \sqrt{\langle \nu | B | \nu \rangle}. \tag{2.9}$$

The linear space S equipped with the norm $\| \, |\nu\rangle \, \|_B$ is a pre-Hilbert space, which can be completed to a Hilbert space with $\langle \mu | B | \nu \rangle$ as its inner product, which will be called the B-Hilbert space. If $B = I$, where I is the identity, the Hilbert space obtained is L^2. If $B = T + \beta^2 I$, where T is the kinetic energy operator and β^2 is a positive real number, the Hilbert space obtained is the first Sobolev space H^1. Other choices of the positive definite operator B give rise to other Hilbert spaces. The basis vectors $|\eta_k\rangle$ satisfy the orthonormality relation

$$\langle \eta_k | B | \eta_\ell \rangle = \delta_{k,\ell}. \tag{2.10}$$

The coefficients $\hat{c}_k$ in (2.5) are determined by minimizing the norm $\| \, |\delta\psi^{(B;K)}\rangle \, \|_B$ of the error $|\delta\psi^{(B;K)}\rangle = |\psi\rangle - |\tilde{\psi}^{(B;K)}\rangle$ to obtain the best approximation in the B-Hilbert space. The result is

$$\hat{c}_k = \langle \eta_k | B | \psi \rangle. \tag{2.11}$$

If the basis vectors $|\eta_k\rangle$ are complete in the B-Hilbert space, the error is given by

$$|\delta\psi^{(B;K)}\rangle = \sum_{k=K+1}^{\infty} \hat{c}_k |\eta_k\rangle. \tag{2.12}$$

The matrix $U_{k,\ell}$ that appears in (2.6) is obtained from the Cholesky decomposition

$$\langle \xi_k | B | \xi_\ell \rangle = B_{k,\ell} = \sum_{j=0}^{\min(k,\ell)} \bar{U}_{j,k} U_{j,\ell}, \tag{2.13}$$

where the bar over $U_{j,k}$ denotes complex conjugation. The $U_{j,\ell}$ are calculated recursively from the formulas

$$U_{k,k} = \left(B_{k,k} - \sum_{j=0}^{k-1} |U_{j,k}|^2 \right)^{1/2}, \tag{2.14}$$

$$U_{k,\ell} = \left(B_{k,\ell} - \sum_{j=0}^{k-1} \bar{U}_{j,k} U_{j,\ell} \right) \Big/ U_{k,k}, \quad k < \ell. \tag{2.15}$$

It should be noted that the construction of the basis vectors $|\eta_k\rangle$ from (2.7), (2.14), and (2.15) guarantees that they are complete in the function space that contains the desired exact wave function $|\psi\rangle$ if the $|\xi_k\rangle$ are complete in that function space, but does not guarantee that they are complete in L^2 or in the B-Hilbert space. This causes no difficulty, however, because only completeness in a function space that contains the desired exact wave function $|\psi\rangle$, and whose notion of convergence implies the convergence of the Rayleigh-Ritz method, is needed for our analysis.

For later use we record the formulas for L^2, which are the $B = I$ special cases of the formulas above. The best approximation in L^2 is $|\psi\rangle \approx |\tilde{\psi}^{(L^2;K)}\rangle$, where

$$|\tilde{\psi}^{(L^2;K)}\rangle = \sum_{k=0}^{K} c_k |\xi_k\rangle. \tag{2.16}$$

The c_k are given for all k by

$$c_k = \langle \xi_k | \psi \rangle. \tag{2.17}$$

The error is

$$|\delta\psi^{(L^2;K)}\rangle = \sum_{k=K+1}^{\infty} c_k |\xi_k\rangle. \tag{2.18}$$

The rate of convergence of the approximation (2.16) can be analyzed by expressing the right-hand side of (2.17) as an integral and using methods for the asymptotic approximation of integrals to obtain a large k asymptotic approximation to c_k. The expansion coefficients $\hat{c}_k$ in the B-Hilbert space are related to the expansion coefficients c_ℓ in L^2 via

$$\hat{c}_k = \sum_{\ell=k}^{\infty} U_{k,\ell} c_\ell. \tag{2.19}$$

Large k asymptotic approximations to the $\hat{c}_k$ can be constructed from (2.19) if asymptotic approximations to $U_{k,\ell}$ and c_k for k and ℓ large are known. It is straightforward to show that the error vectors (2.12) and (2.18) are related by

$$|\delta\psi^{(L^2;K)}\rangle = |\delta\psi^{(B;K)}\rangle + \sum_{k=0}^{K} \sum_{\ell=K+1}^{\infty} U_{k,\ell} c_\ell |\eta_k\rangle. \tag{2.20}$$

An exact formula for the error $\tilde{E}^{(\mathrm{RR};K)} - E$ in the Rayleigh-Ritz approximation to the energy will now be derived via partitioning. Define the projection operators P_K, $\tilde{P}_\parallel$, and $\tilde{P}_\perp$ by

$$P_K = \sum_{k=0}^{K} |\xi_k\rangle\langle\xi_k|, \tag{2.21}$$

$$\tilde{P}_\parallel = |\tilde{\psi}^{(B;K)}\rangle \left(\langle\tilde{\psi}^{(B;K)}|\tilde{\psi}^{(B;K)}\rangle\right)^{-1} \langle\tilde{\psi}^{(B;K)}|, \tag{2.22}$$

$$\tilde{P}_\perp = P_K - \tilde{P}_\parallel. \tag{2.23}$$

Then the matrix eigenvalue problem (2.3) can be written in the partitioned form

$$\tilde{P}_\parallel (H - EI) \tilde{P}_\parallel |\tilde{\psi}^{(\mathrm{RR};K)}\rangle + \tilde{P}_\parallel (H - EI) \tilde{P}_\perp |\tilde{\psi}^{(\mathrm{RR};K)}\rangle = \left(\tilde{E}^{(\mathrm{RR};K)} - E\right) \tilde{P}_\parallel |\tilde{\psi}^{(\mathrm{RR};K)}\rangle, \tag{2.24}$$

$$\tilde{P}_\perp (H - EI) \tilde{P}_\parallel |\tilde{\psi}^{(\mathrm{RR};K)}\rangle + \tilde{P}_\perp (H - EI) \tilde{P}_\perp |\tilde{\psi}^{(\mathrm{RR};K)}\rangle = \left(\tilde{E}^{(\mathrm{RR};K)} - E\right) \tilde{P}_\perp |\tilde{\psi}^{(\mathrm{RR};K)}\rangle. \tag{2.25}$$

Solving Eq. (2.25) for $\tilde{P}_\perp|\tilde{\psi}^{(\mathrm{RR};K)}\rangle$ and inserting the result back in (2.24) yields

$$[\tilde{P}_\parallel (H - EI) \tilde{P}_\parallel - \tilde{P}_\parallel (H - EI) \tilde{P}_\perp A_\perp \tilde{P}_\perp (H - EI) \tilde{P}_\parallel] |\tilde{\psi}^{(\mathrm{RR};K)}\rangle = \left(\tilde{E}^{(\mathrm{RR};K)} - E\right) \tilde{P}_\parallel |\tilde{\psi}^{(\mathrm{RR};K)}\rangle, \tag{2.26}$$

where $A_\perp$ is the generalized inverse (inverse on the subspace that is the span of the range of $\tilde{P}_\perp$) of $\tilde{P}_\perp(H - \tilde{E}^{(\mathrm{RR};K)}I)\tilde{P}_\perp$. The defining equations that specify $A_\perp$ uniquely are

$$A_\perp \left[\tilde{P}_\perp \left(H - \tilde{E}^{(\mathrm{RR};K)} I\right) \tilde{P}_\perp\right] = \left[\tilde{P}_\perp \left(H - \tilde{E}^{(\mathrm{RR};K)} I\right) \tilde{P}_\perp\right] A_\perp = \tilde{P}_\perp, \tag{2.27}$$

$$A_\perp \tilde{P}_\perp = \tilde{P}_\perp A_\perp = A_\perp. \tag{2.28}$$

Define the ordinary inverse $A(\mu)$ by

$$A(\mu) = \left[\tilde{P}_\perp \left(H - \tilde{E}^{(\mathrm{RR};K)} I\right) \tilde{P}_\perp + \mu \tilde{P}_\parallel\right]^{-1} = A_\perp + \mu^{-1} \tilde{P}_\parallel. \tag{2.29}$$

Because $A_\perp = \tilde{P}_\perp A(\mu) \tilde{P}_\perp$, the generalized inverse $A_\perp$ in (2.26) can be replaced by the ordinary inverse $A(\mu)$. Taking the inner product of (2.26) on the left-hand side with $\langle\tilde{\psi}^{(B;K)}|$ yields the error formula

$$\tilde{E}^{(\mathrm{RR};K)} - E = \left[\langle\tilde{\psi}^{(B;K)}| (H - EI) |\tilde{\psi}^{(B;K)}\rangle - \langle\tilde{\psi}^{(B;K)}| (H - EI) \tilde{P}_\perp A(\mu) \tilde{P}_\perp (H - EI) |\tilde{\psi}^{(B;K)}\rangle\right] / \langle\tilde{\psi}^{(B;K)}|\tilde{\psi}^{(B;K)}\rangle. \tag{2.30}$$

The relation

$$(H - EI)\,|\tilde{\psi}^{(B;K)}\rangle = -\,(H - EI)\,|\delta\psi^{(B;K)}\rangle, \tag{2.31}$$

which follows from $(H - EI)\,|\psi\rangle = |0\rangle$, where $|0\rangle$ is the null vector, can be used to bring (2.30) to the form

$$\begin{aligned}\tilde{E}^{(\mathrm{RR};K)} - E = [&\langle\delta\psi^{(B;K)}|\,(H - EI)\,|\delta\psi^{(B;K)}\rangle \\ &-\langle\delta\psi^{(B;K)}|\,(H - EI)\,\tilde{P}_{\perp}A\,(\mu)\,\tilde{P}_{\perp}\,(H - EI)\,|\delta\psi^{(B;K)}\rangle]/\langle\tilde{\psi}^{(B;K)}|\tilde{\psi}^{(B;K)}\rangle.\end{aligned} \tag{2.32}$$

The inverse $A\,(\mu)$, which is needed for the evaluation of the second term in the numerator of (2.32), can be obtained from the generalized Cholesky decomposition

$$\langle\xi_k|\left[\tilde{P}_{\perp}\left(H - \tilde{E}^{(\mathrm{RR};K)}I\right)\tilde{P}_{\perp} + \mu\tilde{P}_{\|}\right]|\xi_\ell\rangle$$

$$= \hat{B}_{k,\ell} = \sum_{j=0}^{\min(k,\ell)} \bar{W}_{j,k}D_{j,j}W_{j,\ell}, \tag{2.33}$$

which is needed because the matrix $\hat{B}_{k,\ell}$ defined by (2.33) is not positive definite for excited states. The $D_{j,j}$, which can take on only the values ±1, and the $W_{j,\ell}$ are calculated recursively from the formulas

$$D_{k,k} = \mathrm{sgn}\left(\hat{B}_{k,k} - \sum_{j=0}^{k-1} D_{j,j}|W_{j,k}|^2\right), \tag{2.34}$$

$$W_{k,k} = \left[D_{k,k}\left(\hat{B}_{k,k} - \sum_{j=0}^{k-1} D_{j,j}|W_{j,k}|^2\right)\right]^{1/2}, \tag{2.35}$$

$$W_{k,\ell} = \left[D_{k,k}\left(\hat{B}_{k,\ell} - \sum_{j=0}^{k-1} \bar{W}_{j,k}D_{j,j}W_{j,\ell}\right)\right] \Big/ W_{k,k}, \quad k < \ell. \tag{2.36}$$

The function sgn, which appears in (2.34), is the sign function: $\mathrm{sgn}\,(x)$ is $+1$ for x positive and -1 for x negative. The elements of the needed inverse $A\,(\mu)$ are given by

$$A_{k,\ell}\,(\mu) = \sum_{j=0}^{\min(k,\ell)} \left(W^{-1}\right)_{k,j} D_{j,j}(\bar{W}^{-1})_{\ell,j}. \tag{2.37}$$

Both $W_{k,\ell}$ and $\left(W^{-1}\right)_{k,\ell}$ are upper triangular matrices.

The computation of error estimates from the exact error formula (2.32) is easier if the positive definite operator B is chosen so that the dominant contributions to the error come from the $\langle\delta\psi^{(B;K)}|\,(H - EI)\,|\delta\psi^{(B;K)}\rangle$ term in the numerator of (2.32). This will happen if the matrix elements $B_{k,\ell} = \langle\xi_k|B|\xi_\ell\rangle$ of the positive definite operator B are approximately equal to the matrix elements $H_{k,\ell} - E\delta_{k,\ell} = \langle\xi_k|\,(H - EI)\,|\xi_\ell\rangle$ for k and ℓ large. If the matrix elements $T_{k,\ell}$ of the kinetic energy are large compared to the matrix elements $V_{k,\ell}$ of the potential energy for k and ℓ large and E is negative, an appropriate choice, which makes the B-Hilbert space the first Sobolev space H^1, is $B = T + \beta^2 I$ with $\beta^2 = -E$. The error estimate for the first example is computed both with this choice and with the choice $B = I$, for which the B-Hilbert space is L^2, so that the reader can see how different choices effect the details of the computation. A suitable B can sometimes be obtained by simply adding a suitable operator S to $H - EI$, with S chosen such that (1) $B = H - EI + S$ is positive definite and (2) the matrix elements $S_{k,\ell}$ of S for k and ℓ large are small compared to the matrix elements $B_{k,\ell}$. This is done for the third model problem (1.10), where E is positive and the choice $S = EI$, which yields $B = H$, is used.

The method described above relates the problem of analyzing rates of convergence for the Rayleigh-Ritz method, which makes the energy expectation value stationary, to the problem of best approximation in a particular Hilbert space, called the B-Hilbert space. The Rayleigh-Ritz expansion coefficients, which change as the size of the basis set increases, are approximated by the coefficients that are obtained by minimizing the distance between the exact and the approximate wave functions in this Hilbert space. An explicit formula [Eq. (2.11)] can be given for these Hilbert space coefficients, which do not change as the size of the basis set increases. The computations that must be performed to implement the method are easiest if the matrix elements of the linear operator B used to define the inner product in the B-Hilbert space are approximately equal asymptotically to the matrix elements of $H - EI$, where H is the Hamiltonian, E is the energy, and I is the identity operator.

III. PROPERTIES OF THE BASIS FUNCTIONS

The basis functions $e_k\,(\alpha; z)$ are normalized so that

$$\int_{-\infty}^{\infty} e_k\,(\alpha; z)\,e_\ell\,(\alpha; z)\;dz = \delta_{k,\ell}. \tag{3.1}$$

The kinetic energy matrix elements are obtained from (3.1) above and

$$\begin{aligned}-\frac{1}{2}\frac{d^2}{dz^2}e_k\,(\alpha; z) = \tfrac{1}{4}\alpha^2\{&-[(k+2)\,(k+1)]^{1/2}\,e_{k+2}\,(\alpha; z) \\ &+(2k+1)\,e_k\,(\alpha; z) \\ &-[k\,(k-1)]^{1/2}\,e_{k-2}\,(\alpha; z)\}.\end{aligned} \tag{3.2}$$

It is convenient to make the definitions

$$e_k^{(+)}(\alpha;z) = \pi^{-3/4}2^{-1/2}(k!)^{1/2}\alpha^{1/2}(-i)^k \times D_{-k-1}\left(-i2^{1/2}\alpha z\right), \quad (3.3)$$

$$e_k^{(-)}(\alpha;z) = \pi^{-3/4}2^{-1/2}(k!)^{1/2}\alpha^{1/2}(i)^k \times D_{-k-1}\left(i2^{1/2}\alpha z\right), \quad (3.4)$$

where the D_{-k-1} are parabolic cylinder functions in standard notation (see [11], pp. 115–132, or [12], pp. 323–335). The functions $e_k^{(+)}(\alpha;z)$ and $e_k^{(-)}(\alpha;z)$ satisfy the same second-order differential equation as $e_k(\alpha;z)$. Their relation to $e_k(\alpha;z)$ is [see [11], p. 117, Eqs. (6) and (9), or [12], p. 325, the first and the fourth equations]

$$e_k(\alpha;z) = e_k^{(+)}(\alpha;z) + e_k^{(-)}(\alpha;z). \quad (3.5)$$

The functions $e_k(\alpha;z)$, $e_k^{(+)}(\alpha;z)$, and $e_k^{(-)}(\alpha;z)$ are all entire functions of z. The large z asymptotic behavior of these functions is given by [see [11], p. 123, Eqs. (2) and (3), or [12], p. 332]

$$e_k(\alpha;z) = \pi^{-1/4}2^{k/2}(k!)^{-1/2}\alpha^{k+1/2}z^k\exp\left(-\alpha^2z^2/2\right)\left[1+O\left(z^{-2}\right)\right]$$
$$\text{for } |z|\to\infty \text{ with } \arg(z) \text{ unrestricted}, \quad (3.6)$$

$$e_k^{(\pm)}(\alpha;z) = \pm i\pi^{-3/4}2^{-(k+2)/2}(k!)^{1/2}\alpha^{-k-1/2}z^{-k-1}\exp\left(\alpha^2z^2/2\right)\left[1+O\left(z^{-2}\right)\right]$$
$$\text{for } |z|\to\infty \text{ with } \arg(z) \text{ restricted to } -\pi/4<\arg(z)<5\pi/4 \text{ for } e_k^{(+)}(\alpha;z)$$
$$\text{and to } -5\pi/4<\arg(z)<\pi/4 \text{ for } e_k^{(-)}(\alpha;z). \quad (3.7)$$

In order to implement the machinery of Sec. II for analyzing the convergence behavior of the Rayleigh-Ritz approximation to the energy, it is necessary to perform a large k asymptotic evaluation of the inner product c_k of the basis function with the exact wave function. This will be done by writing this inner product as an integral, deforming the contour of integration, and using appropriate large k asymptotic approximations to the basis functions $e_k(\alpha;z)$ and the auxiliary functions $e_k^{(\pm)}(\alpha;z)$. A number of different large k expansions for these functions can be obtained from results that are available in the literature; each has been established under a different set of restrictions on α and z. The simplest of these expansions is [see [16], p. 689, Eqs. (19.9.1) and (19.9.3)]

$$e_k^{(\pm)}(\alpha;z) = (2\pi)^{-1/2}(2k+1)^{-1/4}\alpha^{1/2}(\mp i)^k\exp\left[\pm i(2k+1)^{1/2}\alpha z\right] \times\left[1\mp\frac{i\alpha^3z^3}{6(2k+1)^{1/2}}+\frac{1}{(2k+1)}\left(\frac{\alpha^2z^2}{4}-\frac{\alpha^6z^6}{72}\right)\pm\frac{i}{(2k+1)^{3/2}}\left(\frac{\alpha z}{4}-\frac{\alpha^5z^5}{15}+\frac{\alpha^9z^9}{1296}\right)+O\left(k^{-2}\right)\right]. \quad (3.8)$$

Expansion (3.8) is valid for k large and z moderate (i.e., z bounded as k tends to infinity).

Expansions valid in a larger domain in the complex z plane can be obtained by trying to approximate the functions e_k and $e_k^{(\pm)}$ with the aid of "qualitatively similar" functions. The simplest approximation of this type is the Liouville-Green formula $q^{-1/2}\exp\left(\pm i\int qdz\right)$ for the approximate solution of the differential equation $f''+q^2f=0$, which is familiar from the WKB method. The exponential function is the qualitatively similar function in this case. The formulas obtained with the aid of the Liouville-Green approximation and its systematic extension to higher order yield the following expansions [17], which are valid in a larger domain:

$$e_k(\alpha;z) = (2\pi)^{-1/2}(2k+1)^{-1/4}\alpha^{1/2}\left(t^2-1\right)^{-1/4} \times\exp\left[-(2k+1)\xi(t)\right] \times\left[1+\frac{t^3-6t}{24(2k+1)\left(t^2-1\right)^{3/2}}+O\left(k^{-2}\right)\right], \quad (3.9)$$

$$e_k^{(\pm)}(\alpha;z) = \pm i(2\pi)^{-1/2}(2k+1)^{-1/4} \times\alpha^{1/2}(t^2-1)^{-1/4}\exp[(2k+1)\xi(t)] \times\left[1-\frac{t^3-6t}{24(2k+1)(t^2-1)^{3/2}} +O(k^{-2})\right], \quad (3.10)$$

where

$$\xi(t) = \tfrac{1}{2}t\sqrt{t^2-1} - \tfrac{1}{2}\ln\left(t+\sqrt{t^2-1}\right), \quad (3.11)$$

with

$$t = \alpha z/\sqrt{2k+1}. \quad (3.12)$$

The expansion (3.9) is Eq. (4.3) of [17] with $\mu = \sqrt{2k+1}$; (3.10) is Eq. (4.3) of [17] with $\mu = -i\sqrt{2k+1}$ for $e_k^{(+)}(\alpha;z)$ and $\mu = i\sqrt{2k+1}$ for $e_k^{(-)}(\alpha;z)$. The domains of validity of (3.9) and (3.10) are described in detail in [17] [see Fig. 2 of [17] pictures (a) and (c)]. For our purposes it is sufficient to note that (3.9) is uniformly valid in t for k large if t is in the right half of the complex t plane and a finite distance away from a line that runs from -1 to 1 along the real t axis, that (3.10) applied to $e_k^{(+)}(\alpha;z)$ is uniformly valid in t for k large if t is in the upper half of the complex t plane and a finite distance away from the turning points at $+1$ and at -1, and that (3.10) applied to $e_k^{(-)}(\alpha;z)$ is uniformly valid in t for k large if t is in the lower half of the complex t plane and a finite distance away from the turning points at $+1$ and at -1 (the turning points are the points where the q in the Liouville-Green formula has a zero). The asymptotic expansion (3.10) applied to $e_k^{(+)}(\alpha;z)$ differs from the asymptotic expansion (3.10) applied to $e_k^{(-)}(\alpha;z)$ only in overall sign because the exponentially growing pieces of $e_k^{(+)}(\alpha;z)$ and $e_k^{(-)}(\alpha;z)$ must cancel when $e_k^{(+)}(\alpha;z)$ and $e_k^{(-)}(\alpha;z)$ are combined in (3.5) to obtain the exponentially decaying $e_k(\alpha;z)$.

The Liouville-Green formula breaks down at the turning points for the basis functions, which lie at the points

$$\pm x_k^{(0)} = \pm(2k+1)^{1/2}\alpha^{-1}, \quad (3.13)$$

which are the images of the points $t = \pm 1$ under the change of variables (3.12). The breakdown occurs because the behavior of the functions e_k and $e_k^{(\pm)}$ changes from oscillatory to exponential as one moves along the real axis through a turning point. The simplest qualitatively similar function that exhibits such a change is the Airy function. For this reason the asymptotic expansions that remain valid at the turning points are based on Airy functions instead of exponential functions. The following expansions in Airy functions [17] are valid in a domain that includes the neighborhood of the turning point $t = 1$ where (3.9) and (3.10) break down:

$$e_k(\alpha;z) = 2^{1/2}(2k+1)^{-1/12}\alpha^{1/2}\left(\frac{\zeta}{t^2-1}\right)^{1/4} \times[\mathrm{Ai}(y_0) + (2k+1)^{-4/3}B_0(\zeta)\mathrm{Ai}'(y_0) +O(k^{-2})], \quad (3.14)$$

$$e_k^{(\pm)}(\alpha;z) = 2^{1/2}(2k+1)^{-1/12}\alpha^{1/2} \times\exp(\pm i\pi/3)\left(\frac{\zeta}{t^2-1}\right)^{1/4} \times[\mathrm{Ai}(y_\pm) + (2k+1)^{-4/3}\exp(\mp 2\pi i/3) \times B_0(\zeta)\mathrm{Ai}'(y_\pm) + O(k^{-2})], \quad (3.15)$$

where

$$\zeta = \left[\tfrac{3}{2}\xi(t)\right]^{2/3}, \quad (3.16)$$

$$y_0 = (2k+1)^{2/3}\zeta, \quad (3.17)$$

$$y_\pm = \exp(\mp 2\pi i/3)\, y_0, \quad (3.18)$$

and

$$B_0(\zeta) = -\zeta^{-1/2}\left[\frac{t^3-6t}{24(t^2-1)^{3/2}} + \frac{5}{72\xi(t)}\right]. \quad (3.19)$$

Individual terms on the right-hand side of (3.19) are singular at $t = 1$. However, the expansion of this right-hand side about $t = 1$ shows that the singular terms cancel. The function $B_0(\zeta)$ is actually an analytic function of t in the neighborhood of $t = 1$, with the expansion

$$B_0(\zeta) = -\frac{9}{280}2^{1/3} + \frac{7}{450}2^{1/3}(t-1) + O\left[(t-1)^2\right] \quad (3.20)$$

about $t = 1$. The expansion (3.14) is Eq. (8.11) of [17] with $\mu = \sqrt{2k+1}$; (3.15) is Eq. (8.11) of [17] with $\mu = -i\sqrt{2k+1}$ for $e_k^{(+)}(\alpha;z)$ and $\mu = i\sqrt{2k+1}$ for $e_k^{(-)}(\alpha;z)$. The domains of validity of (3.14) and (3.15) are also described in detail in [17] [see Fig. 7 of [17] pictures (a) and (c)]. For our purposes it is sufficient to note that (3.14) and (3.15) are uniformly valid in t for k large if t is in the right half of the complex t plane and otherwise unrestricted.

The expansions listed above form a hierarchy in which the description of ever more complicated behavior is made possible by using functions of increasing complexity. Expansions (3.9) and (3.10) can be obtained from (3.14) and (3.15) by using asymptotic expansions for the Airy function and its derivative. Similarly (3.8) can be obtained from (3.10) by making a small t expansion. The large k expansions of (3.6) and (3.7) obtained by using the Stirling approximation to the factorial agree with the large z expansions of (3.9) and (3.10). These interrelated expansions provide the descriptions of the functions $e_k(\alpha;z)$, $e_k^{(+)}(\alpha;z)$, and $e_k^{(-)}(\alpha;z)$ in terms of simpler functions that will be needed in Secs. IV, V, and VI for the construction of large k asymptotic expansions of the expansion coefficients c_k that are uniformly valid in α.

One of the contributions to the large k asymptotic behavior of the c_k in the examples of Secs. IV and V comes from the neighborhood of the classical turning points (3.13) for the basis functions $e_k(\alpha;x)$. The needed turning point contributions are

$$c_k^{(\mathrm{TP},+)} = \int_{+i\infty}^{x_k^{(0)}} e_k^{(+)}(\alpha;z)\,\psi(z)\,dz + \int_{-i\infty}^{x_k^{(0)}} e_k^{(-)}(\alpha;z)\,\psi(z)\,dz + \int_{x_k^{(0)}}^{\infty} e_k(\alpha;z)\,\psi(z)\,dz, \tag{3.21}$$

$$c_k^{(\mathrm{TP},-)} = \int_{-\infty}^{-x_k^{(0)}} e_k(\alpha;z)\,\psi(z)\,dz + \int_{-x_k^{(0)}}^{+i\infty} e_k^{(+)}(\alpha;z)\,\psi(z)\,dz + \int_{-x_k^{(0)}}^{-i\infty} e_k^{(-)}(\alpha;z)\,\psi(z)\,dz. \tag{3.22}$$

An asymptotic expansion of the turning point contribution $c_k^{(\mathrm{TP},+)}$ can be obtained by expanding the wave function $\psi(z)$ in Taylor series about the turning point $x_k^{(0)}$, replacing $e_k(\alpha;z)$ and $e_k^{(\pm)}(\alpha;z)$ by the Airy function asymptotic approximations (3.14) and (3.15) and integrating term by term. The result is

$$\begin{aligned} c_k^{(\mathrm{TP},+)} = {} & \alpha^{-1/2}(2k+1)^{-1/4}\Big\{\psi\left(x_k^{(0)}\right) + \tfrac{1}{6}\alpha^{-3}\psi^{(3)}\left(x_k^{(0)}\right)(2k+1)^{-1/2} \\ & + \left[-\tfrac{1}{4}\alpha^{-2}\psi^{(2)}\left(x_k^{(0)}\right) + \tfrac{1}{72}\alpha^{-6}\psi^{(6)}\left(x_k^{(0)}\right)\right](2k+1)^{-1} + \left[\tfrac{1}{4}\alpha^{-1}\psi^{(1)}\left(x_k^{(0)}\right)\right. \\ & \left. - \tfrac{1}{15}\alpha^{-5}\psi^{(5)}\left(x_k^{(0)}\right) + \tfrac{1}{1296}\alpha^{-9}\psi^{(9)}\left(x_k^{(0)}\right)\right](2k+1)^{-3/2} + O\left(k^{-2}\right)\Big\}, \end{aligned} \tag{3.23}$$

where $\psi^{(j)}(x_k^{(0)})$ is the value of the jth derivative of ψ at $x_k^{(0)}$. The derivation of (3.23) assumes that the exponential decay of the Airy function in the asymptotic approximations (3.14) and (3.15) cuts off the integrals fast enough so that only the neighborhood of the turning point $x_k^{(0)}$ makes a significant contribution to the integrals. It is valid if the wave function ψ varies slowly in this neighborhood. A similar calculation yields

$$\begin{aligned} c_k^{(\mathrm{TP},-)} = {} & (-1)^k\alpha^{-1/2}(2k+1)^{-1/4}\Big\{\psi\left(-x_k^{(0)}\right) + \tfrac{1}{6}\alpha^{-3}\psi^{(3)}\left(-x_k^{(0)}\right)(2k+1)^{-1/2} \\ & + \left[-\tfrac{1}{4}\alpha^{-2}\psi^{(2)}\left(-x_k^{(0)}\right) + \tfrac{1}{72}\alpha^{-6}\psi^{(6)}\left(-x_k^{(0)}\right)\right](2k+1)^{-1} + \left[\tfrac{1}{4}\alpha^{-1}\psi^{(1)}\left(-x_k^{(0)}\right)\right. \\ & \left. - \tfrac{1}{15}\alpha^{-5}\psi^{(5)}\left(-x_k^{(0)}\right) + \tfrac{1}{1296}\alpha^{-9}\psi^{(9)}\left(-x_k^{(0)}\right)\right](2k+1)^{-3/2} + O\left(k^{-2}\right)\Big\} \end{aligned} \tag{3.24}$$

for the contribution from the neighborhood of the turning point $-x_k^{(0)}$. Formula (3.24) can be derived from (3.23) with the aid of the reflection $z \to -z$, which interchanges $c_k^{(\mathrm{TP},+)}$ and $c_k^{(\mathrm{TP},-)}$.

IV. THE $\cosh^{-2}$ POTENTIAL

The Hamiltonian (1.8) is one of the small number of examples for which the Schrödinger equation can be solved exactly (see [18], pp. 69–70, Problem 4). This Hamiltonian has been chosen as the first example because it illustrates particularly clearly the way in which the optimum value of α can be determined by a competition between contributions from singularities of the wave function and contributions from the neighborhoods of the classical turning points of the basis functions. The exact ground state energy E_0 and wave function $\psi(x)$ for this Hamiltonian are

$$E_0 = -\tfrac{1}{2} \tag{4.1}$$

and

$$\psi(x) = \frac{1}{\sqrt{2}\cosh(x)}. \tag{4.2}$$

The rate of convergence of Rayleigh-Ritz approximations to the ground state energy (4.1) will be analyzed for a variational trial function of the form

$$\tilde{\psi}^{(\mathrm{RR};K)}(x) = \sum_{k=0}^{K} \tilde{c}_k^{(\mathrm{RR};K)} e_{2k}(\alpha;x). \tag{4.3}$$

The exact expansion coefficients c_k to which the $\tilde{c}_k^{(\mathrm{RR};K)}$ converge as $K \to \infty$ are given by

$$c_k = \int_{-\infty}^{\infty} e_{2k}(\alpha;x)\,\psi(x)\,dx. \tag{4.4}$$

The $k \to \infty$ asymptotic behavior of c_k will be extracted by using (3.5) to rewrite (4.4) in the form

$$c_k = c_k^{(1)} + c_k^{(2)} + c_k^{(3)} + c_k^{(4)}, \tag{4.5}$$

where

$$c_k^{(1)} = \int_{-\infty}^{-x_{2k}^{(0)}} e_{2k}(\alpha; x)\,\psi(x)\,dx, \tag{4.6}$$

$$c_k^{(2)} = \int_{-x_{2k}^{(0)}}^{x_{2k}^{(0)}} e_{2k}^{(+)}(\alpha; x)\,\psi(x)\,dx, \tag{4.7}$$

$$c_k^{(3)} = \int_{-x_{2k}^{(0)}}^{x_{2k}^{(0)}} e_{2k}^{(-)}(\alpha; x)\,\psi(x)\,dx, \tag{4.8}$$

$$c_k^{(4)} = \int_{x_{2k}^{(0)}}^{\infty} e_{2k}(\alpha; x)\,\psi(x)\,dx. \tag{4.9}$$

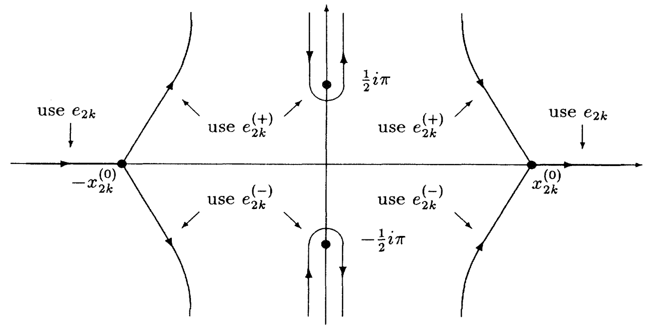

FIG. 1. Integration contours for the $\cosh^{-2}$ potential.

The integration contours are deformed as shown in Fig. 1. Because $e_{2k}^{(+)}(\alpha; z)$ decays exponentially to zero as z moves off to infinity in the upper half of the complex z plane, it is convenient to deform the integration contour in (4.7) into the upper half plane. Similarly, the exponential decay of $e_{2k}^{(-)}(\alpha; z)$ as z tends to infinity in the lower half plane makes it convenient to deform the integration contour in (4.8) into the lower half plane. The integration contour for $c_k^{(2)}$ is pulled into the upper half plane to obtain a piece from $-x_{2k}^{(0)}$ to $+i\infty$, plus a loop that starts at $+i\infty$, runs around the poles of ψ on the imaginary axis, and goes back to $+i\infty$, plus a piece from $+i\infty$ to $x_{2k}^{(0)}$. The integration contour for $c_k^{(3)}$ is pulled into the lower half plane to obtain a piece from $-x_{2k}^{(0)}$ to $-i\infty$, plus a loop that starts at $-i\infty$, runs around the poles of ψ on the imaginary axis, and goes back to $-i\infty$, plus a piece from $-i\infty$ to $x_{2k}^{(0)}$. These contour deformations are justified by Cauchy's theorem, the exponential falloff of the $e_{2k}^{(\pm)}(\alpha; z)$, and the fact that the only singularities of the integrand are the poles of ψ at the zeros of $\cosh(z)$ on the imaginary axis. The contributions from the loops around the poles of ψ on the imaginary axis are combined to give the term $c_k^{(\text{sing})}$, which comes from the singularities of the wave function. The contributions from the contours that run from $-x_{2k}^{(0)}$ to $\pm i\infty$ are combined with $c_k^{(1)}$ to give a turning point contribution $c_{2k}^{(\text{TP},-)}$ of the form (3.22). The contributions from the contours that run from $\pm i\infty$ to $x_{2k}^{(0)}$ are combined with $c_k^{(4)}$ to give a turning point contribution $c_{2k}^{(\text{TP},+)}$ of the form (3.21).

The singularities contribution $c_k^{(\text{sing})}$ is dominated by the poles nearest the real axis (at $\pm i\pi/2$) for k large; computing the residue at these poles and using the asymptotic approximation (3.8) yields

$$\begin{aligned} c_k^{(\text{sing})} &= 2(\pi\alpha)^{1/2}(4k+1)^{-1/4}(-1)^k \exp\left[-\tfrac{1}{2}\pi\alpha(4k+1)^{1/2}\right] \\ &\quad\times\Big\{1 - \tfrac{1}{48}(\pi\alpha)^3(4k+1)^{-1/2} - \tfrac{1}{16}(\pi\alpha)^2\left[1 - \tfrac{1}{288}(\pi\alpha)^4\right](4k+1)^{-1} \\ &\quad - \tfrac{1}{8}\pi\alpha\left[1 - \tfrac{1}{60}(\pi\alpha)^4 + \tfrac{1}{82\,944}(\pi\alpha)^8\right](4k+1)^{-3/2} + O\left(k^{-2}\right)\Big\}. \end{aligned} \tag{4.10}$$

We denote the sum of the turning point contributions $c_{2k}^{(\text{TP},+)}$ and $c_{2k}^{(\text{TP},-)}$ by $c_k^{(\text{TP})}$ and evaluate it with the aid of (3.23), (3.24), and the approximation $\psi(\pm x) \approx \sqrt{2}\exp(\mp x)$. The result is

$$\begin{aligned} c_k^{(\text{TP})} &= 2^{3/2}\alpha^{-1/2}(4k+1)^{-1/4}\exp\left[-\alpha^{-1}(4k+1)^{1/2}\right]\{1 - \tfrac{1}{6}\alpha^{-3}(4k+1)^{-1/2} \\ &\quad - \left[\tfrac{1}{4}\alpha^{-2} - \tfrac{1}{72}\alpha^{-6}\right](4k+1)^{-1} - \left[\tfrac{1}{4}\alpha^{-1} - \tfrac{1}{15}\alpha^{-5} + \tfrac{1}{1296}\alpha^{-9}\right](4k+1)^{-3/2} + O\left(k^{-2}\right)\}. \end{aligned} \tag{4.11}$$

A large K asymptotic approximation to $\tilde{E}^{(\text{RR};K)} - E$ can be obtained from (2.32). The result has the form

$$\tilde{E}^{(\text{RR};K)} - E = \tilde{E}_K^{(\text{sing})} + \tilde{E}_K^{(\text{TP})} + (-1)^{K+1}\tilde{E}_K^{(\text{cross})}, \tag{4.12}$$

where $\tilde{E}_K^{(\text{sing})}$ is the singularities contribution from (4.10), $\tilde{E}_K^{(\text{TP})}$ is the turning point contribution from (4.11), and $(-1)^{K+1}\tilde{E}_K^{(\text{cross})}$ is the cross term between the singularities and turning point contributions. The alternating sign $(-1)^{K+1}$ that appears in the cross term arises because the $c_k^{(\text{sing})}$ alternate in sign due to the factor $(-1)^k$ in (4.10) while the $c_k^{(\text{TP})}$ are all positive. This alternating sign in the cross term is an interference effect between the singularities and the turning point contributions. The explicit formulas for these three contributions are

$$\tilde{E}_K^{(\mathrm{sing})} = \alpha^2 (4K+5) \exp\left[-\pi\alpha (4K+5)^{1/2}\right] \left\{1 + \left[2(\pi\alpha)^{-1} - \tfrac{1}{24}(\pi\alpha)^3\right](4K+5)^{-1/2} + \left[\left(2\pi^{-2}+1\right)\alpha^{-2} + \pi - \tfrac{1}{12}(\pi\alpha)^2 + \tfrac{1}{1152}(\pi\alpha)^6 - \frac{4}{\pi^2\alpha}\zeta\left(2, \tfrac{1}{2}\alpha + \tfrac{1}{2}\right)\right](4K+5)^{-1} + O\left(K^{-3/2}\right)\right\}, \quad (4.13)$$

$$\tilde{E}_K^{(\mathrm{TP})} = 4\exp\left[-2\alpha^{-1}(4K+5)^{1/2}\right]\left\{1 - \tfrac{1}{3}\alpha^{-3}(4K+5)^{-1/2} + \tfrac{1}{18}\alpha^{-6}(4K+5)^{-1} + O\left(K^{-3/2}\right)\right\}, \quad (4.14)$$

$$\tilde{E}_K^{(\mathrm{cross})} = 2^{5/2}\pi^{1/2}\alpha \exp\left[-\left(\tfrac{1}{2}\pi\alpha + \alpha^{-1}\right)(4K+5)^{1/2}\right]\left\{1 - \left[\tfrac{1}{6}\alpha^{-3} + \tfrac{1}{48}(\pi\alpha)^3\right](4K+5)^{-1/2} + O\left(K^{-1}\right)\right\}. \quad (4.15)$$

The function $\zeta\left(2, \frac{1}{2}\alpha + \frac{1}{2}\right)$, which appears in (4.13), is the Hurwitz zeta function, also known as the generalized zeta function, in standard notation (see [12], pp. 22–25, or [19], pp. 24–27). The derivation of (4.12)–(4.15) from (2.32) can be carried out by using either the best approximation $|\tilde{\psi}^{(L^2;K)}\rangle$ in L^2 or the best approximation $|\tilde{\psi}^{(H^1;K)}\rangle$ in H^1 for $|\tilde{\psi}^{(K)}\rangle$. The derivation is easiest if $|\tilde{\psi}^{(H^1;K)}\rangle$ is used, because $|\tilde{\psi}^{(H^1;K)}\rangle$ is closer to the Rayleigh-Ritz approximation $|\tilde{\psi}^{(\mathrm{RR};K)}\rangle$ than $|\tilde{\psi}^{(L^2;K)}\rangle$. Computational details and a comparison of these two ways of deriving (4.12)–(4.15) can be found in Appendix A below. Table I compares the exact value of the error $\delta E_R = \tilde{E}^{(\mathrm{RR};K)} - E$ obtained by performing the Rayleigh-Ritz calculation with the asymptotic approximation for three different values of α, namely, $\alpha = 0.5$, $\alpha = 0.8$, and $\alpha = 0.11$. The asymptotic approximation δE_A to δE_R is given by the right-hand side of (4.12), with the terms given by (4.13)–(4.15). The table lists the relative error $\delta^2 E/\delta E_R = (\delta E_R - \delta E_A)/\delta E_R$ for $\alpha = 0.5$, where $\tilde{E}_K^{(\mathrm{sing})}$ is the dominant contribution, for

TABLE I. The exact error δE_R and the relative error $(\delta E_R - \delta E_A)/\delta E_R = \delta^2 E/\delta E_R$ in the approximation δE_A to δE_R for the $\cosh^{-2}$ potential.

	$\alpha = 0.5$		$\alpha = 0.8$		$\alpha = 0.11$	
K	δE_R	$\delta^2 E/\delta E_R$	δE_R	$\delta^2 E/\delta E_R$	δE_R	$\delta^2 E/\delta E_R$
0	8.2×10^{-2}	-1.5×10^{-1}	9.9×10^{-3}	-1.5×10^{-1}	4.6×10^{-2}	-3.9×10^{-2}
1	3.9×10^{-2}	-5.7×10^{-2}	9.3×10^{-3}	-4.1×10^{-2}	1.9×10^{-2}	9.3×10^{-3}
2	1.9×10^{-2}	-5.2×10^{-2}	8.8×10^{-4}	-3.1×10^{-2}	4.8×10^{-3}	-3.7×10^{-3}
3	1.0×10^{-2}	-3.9×10^{-2}	7.5×10^{-4}	-2.3×10^{-2}	2.3×10^{-3}	-3.8×10^{-3}
4	5.7×10^{-3}	-3.3×10^{-2}	1.3×10^{-4}	-1.5×10^{-2}	8.6×10^{-4}	-3.7×10^{-3}
5	3.4×10^{-3}	-2.7×10^{-2}	1.0×10^{-4}	-1.4×10^{-2}	4.4×10^{-4}	-3.8×10^{-3}
6	2.1×10^{-3}	-2.3×10^{-2}	2.4×10^{-5}	-9.2×10^{-3}	2.1×10^{-4}	-3.0×10^{-3}
7	1.3×10^{-3}	-2.0×10^{-2}	1.9×10^{-5}	-9.7×10^{-3}	1.1×10^{-4}	-2.9×10^{-3}
8	8.6×10^{-4}	-1.8×10^{-2}	5.3×10^{-6}	-6.5×10^{-3}	5.9×10^{-5}	-2.3×10^{-3}
9	5.7×10^{-4}	-1.6×10^{-2}	4.1×10^{-6}	-7.2×10^{-3}	3.4×10^{-5}	-2.1×10^{-3}
10	3.8×10^{-4}	-1.4×10^{-2}	1.3×10^{-6}	-4.9×10^{-3}	1.9×10^{-5}	-1.8×10^{-3}
20	1.3×10^{-5}	-7.1×10^{-3}	4.6×10^{-9}	-2.1×10^{-3}	2.0×10^{-7}	-6.8×10^{-4}
30	8.4×10^{-7}	-4.7×10^{-3}	5.0×10^{-11}	-1.3×10^{-3}	5.8×10^{-9}	-3.7×10^{-4}
40	8.0×10^{-8}	-3.5×10^{-3}	1.0×10^{-12}	-8.9×10^{-4}	2.8×10^{-10}	-2.4×10^{-4}
50	9.7×10^{-9}	-2.9×10^{-3}	3.1×10^{-14}	-6.7×10^{-4}	1.9×10^{-11}	-1.7×10^{-4}
60	1.4×10^{-9}	-2.4×10^{-3}	1.3×10^{-15}	-5.4×10^{-4}	1.7×10^{-12}	-1.3×10^{-4}
70	2.3×10^{-10}	-2.1×10^{-3}	6.8×10^{-17}	-4.5×10^{-4}	1.8×10^{-13}	-1.0×10^{-4}
80	4.4×10^{-11}	-1.8×10^{-3}	4.4×10^{-18}	-3.8×10^{-4}	2.3×10^{-14}	-8.2×10^{-5}
90	9.1×10^{-12}	-1.6×10^{-3}	3.3×10^{-19}	-3.3×10^{-4}	3.2×10^{-15}	-6.9×10^{-5}
91	7.8×10^{-12}	-1.6×10^{-3}	2.7×10^{-19}	-3.7×10^{-4}	2.7×10^{-15}	-6.8×10^{-5}
92	6.7×10^{-12}	-1.6×10^{-3}	2.0×10^{-19}	-3.2×10^{-4}	2.2×10^{-15}	-6.7×10^{-5}
93	5.7×10^{-12}	-1.6×10^{-3}	1.7×10^{-19}	-3.6×10^{-4}	1.8×10^{-15}	-6.5×10^{-5}
94	4.9×10^{-12}	-1.5×10^{-3}	1.2×10^{-19}	-3.1×10^{-4}	1.5×10^{-15}	-6.4×10^{-5}
95	4.2×10^{-12}	-1.5×10^{-3}	1.0×10^{-19}	-3.5×10^{-4}	1.3×10^{-15}	-6.3×10^{-5}
96	3.6×10^{-12}	-1.5×10^{-3}	7.4×10^{-20}	-3.1×10^{-4}	1.1×10^{-15}	-6.2×10^{-5}
97	3.1×10^{-12}	-1.5×10^{-3}	6.2×10^{-20}	-3.4×10^{-4}	8.8×10^{-16}	-6.1×10^{-5}
98	2.7×10^{-12}	-1.5×10^{-3}	4.5×10^{-20}	-3.0×10^{-4}	7.3×10^{-16}	-6.0×10^{-5}
99	2.3×10^{-12}	-1.5×10^{-3}	3.8×10^{-20}	-3.3×10^{-4}	6.1×10^{-16}	-5.9×10^{-5}
100	2.0×10^{-12}	-1.4×10^{-3}	2.8×10^{-20}	-2.9×10^{-4}	5.1×10^{-16}	-5.9×10^{-5}

$\alpha = 0.11$, where $\tilde{E}_K^{(\mathrm{TP})}$ is the dominant contribution, and for $\alpha = 0.8$, where the terms $\tilde{E}_K^{(\mathrm{sing})}$ and $\tilde{E}_K^{(\mathrm{TP})}$ are comparable, with $\tilde{E}_K^{(\mathrm{cross})}$, which contains the interference effect, making a smaller but still noticeable contribution. The asymptotic approximation follows the error surprisingly well; even for K as small as 10, the relative error in the asymptotic approximations δE_A to δE_R is 1.5% or less.

The asymptotic approximation (4.12)–(4.15) for the error can be optimized with respect to the nonlinear parameter α to obtain an asymptotic approximation to the value $\alpha_{\mathrm{opt}}(K)$ that yields the best approximation to the energy for a given value of K. The lowest-order result is

$$\alpha_{\mathrm{opt}}(K) = \left(\frac{2}{\pi}\right)^{1/2} + O\left[K^{-1/2}\ln(K)\right]. \qquad (4.16)$$

This $(2/\pi)^{1/2}$ leading term in the large K expansion $\alpha_{\mathrm{opt}}(K)$ makes the exponential factors $\exp[-\pi\alpha(4N+5)^{1/2}]$ in (4.13), $\exp[-2\alpha^{-1}(4K+5)^{1/2}]$ in (4.14), and $\exp[-(\frac{1}{2}\pi\alpha+\alpha^{-1})(4K+5)^{1/2}]$ in (4.15) equal. Carrying the expansion to higher order yields

$$\alpha_{\mathrm{opt}}(K) = \left(\frac{2}{\pi}\right)^{1/2}\Bigg\{1+\sum_{\ell=1}^{3}\alpha_{\mathrm{opt}}^{(\ell)}(K)\left[2\pi(4K+5)\right]^{-\ell/2} + (-1)^{K+1}\beta_{\mathrm{opt}}^{(3)}(K)\left[2\pi(4K+5)\right]^{-3/2} + O\left(K^{-2}\right)\Bigg\}, \qquad (4.17)$$

where $\beta_{\mathrm{opt}}^{(3)}(K)$ and the $\alpha_{\mathrm{opt}}^{(\ell)}(K)$, which have a weak logarithmic dependence on K, are given by

$$\alpha_{\mathrm{opt}}^{(1)}(K) = \tfrac{1}{2}\ln\left(\frac{4K+5}{2\pi}\right), \qquad (4.18)$$

$$\alpha_{\mathrm{opt}}^{(2)}(K) = \tfrac{1}{8}\ln^2\left(\frac{4K+5}{2\pi}\right) + \ln\left(\frac{4K+5}{2\pi}\right), \qquad (4.19)$$

$$\alpha_{\mathrm{opt}}^{(3)}(K) = \tfrac{1}{2}\ln^2\left(\frac{4K+5}{2\pi}\right) + \left(2-\tfrac{1}{4}\pi^2\right)\ln\left(\frac{4K+5}{2\pi}\right) + \tfrac{3}{2}\pi^2 - 4(2\pi)^{-1/2}\zeta\left[2,(2\pi)^{-1/2}+\tfrac{1}{2}\right], \qquad (4.20)$$

$$\beta_{\mathrm{opt}}^{(3)}(K) = \pi\left[\ln\left(\frac{4K+5}{2\pi}\right) - 2\right]. \qquad (4.21)$$

The $\alpha_{\mathrm{opt}}^{(1)}(K)(4K+5)^{-1/2}$ first correction makes both $\tilde{E}_K^{(\mathrm{sing})}$ and $\tilde{E}_K^{(\mathrm{TP})}$ have the value $2^{3/2}\pi^{-1/2}(4K+5)^{1/2}\exp\{-[2\pi(4K+5)]^{1/2}\}$ to leading order for K large. It is interesting to note that the interference effect between the singularities and turning point contributions [the alternating sign $(-1)^{K+1}$] does not show up until the $(4K+5)^{-3/2}$ term in the expansion; this happens because $\partial\tilde{E}_K^{(\mathrm{cross})}/\partial\alpha$ is smaller than $\partial\tilde{E}_K^{(\mathrm{sing})}/\partial\alpha$ and $\partial\tilde{E}_K^{(\mathrm{TP})}/\partial\alpha$ by a factor of $(4K+5)$ at $\alpha = \alpha_{\mathrm{opt}}(K)$. The error in the energy when α has its optimum value can be obtained by using (4.17)–(4.21) in (4.12)–(4.15). The result is

$$\left[\tilde{E}^{(\mathrm{RR};K)} - E\right]_{\alpha=\alpha_{\mathrm{opt}}(K)} = 8\left(\frac{4K+5}{2\pi}\right)^{1/2}\exp\left\{-\left[2\pi(4K+5)\right]^{1/2}\right\} \times\left[1+\sum_{\ell=1}^{2}\delta E_{\mathrm{opt}}^{(\ell)}(K)\left[2\pi(4K+5)\right]^{-\ell/2} + O\left(N^{-3/2}\right)\right], \qquad (4.22)$$

where the $\delta E_{\mathrm{opt}}^{(\ell)}(K)$, which contain both the $(-1)^{K+1}$ interference effect and a weak logarithmic dependence on K, are given by

$$\delta E_{\mathrm{opt}}^{(1)}(K) = 2\pi(-1)^{K+1} - \tfrac{1}{8}\ln^2\left(\frac{4K+5}{2\pi}\right) + \tfrac{1}{2}\ln\left(\frac{4K+5}{2\pi}\right) + 1 - \tfrac{1}{6}\pi^2, \qquad (4.23)$$

$$\delta E_{\mathrm{opt}}^{(2)}(K) = \pi(-1)^{K+1}\left[-\tfrac{1}{4}\ln^2\left(\frac{4K+5}{2\pi}\right) + \ln\left(\frac{4K+5}{2\pi}\right) - \tfrac{1}{3}\pi^2\right] + \tfrac{1}{128}\ln^4\left(\frac{4K+5}{2\pi}\right) - \tfrac{1}{16}\ln^3\left(\frac{4K+5}{2\pi}\right) + \left(\tfrac{1}{48}\pi^2 - \tfrac{3}{8}\right)\ln^2\left(\frac{4K+5}{2\pi}\right) + \left(\tfrac{1}{2} - \tfrac{1}{12}\pi^2\right)\ln\left(\frac{4K+5}{2\pi}\right) + 1 + \tfrac{4}{3}\pi^2 + \tfrac{1}{72}\pi^4 - 4(2\pi)^{-1/2}\zeta\left[2,(2\pi)^{-1/2}+\tfrac{1}{2}\right]. \qquad (4.24)$$

Table II exhibits exact values of $\alpha_{\mathrm{opt}}(K)$ obtained by numerical optimization of the Rayleigh-Ritz calculation with respect to α and compares them with asymptotic approximations. The quantities tabulated in Table II are defined as follows. $\delta\alpha_1/\alpha$ is the exact value of $\alpha_{\mathrm{opt}}(K)$ minus the asymptotic approximation to $\alpha_{\mathrm{opt}}(K)$ given by (4.17)–(4.21) divided by the exact value of $\alpha_{\mathrm{opt}}(K)$. $\delta\alpha_2/\alpha$ is the exact value of $\alpha_{\mathrm{opt}}(K)$ minus the asymptotic approximation to $\alpha_{\mathrm{opt}}(K)$ obtained by numerical minimization of the energy error expressions (4.12)–(4.15) divided by the exact value of $\alpha_{\mathrm{opt}}(K)$. $\delta^2E_1/\delta E_R$ is the exact error in the energy when $\alpha = \alpha_{\mathrm{opt}}(K)$ minus the asymptotic approximation to this exact error given by (4.22)–(4.24) divided by the exact error. $\delta^2 E_2/\delta E_R$ is the exact error in the energy when $\alpha = \alpha_{\rm opt}(K)$ minus the asymptotic approximation to this exact error when the asymptotic approximation to $\alpha_{\rm opt}(K)$ obtained by numerical minimization of the energy error expressions (4.12)–(4.15) divided by the exact error. It is readily apparent that the errors are smaller when the asymptotic approximation to $\alpha_{\rm opt}(K)$ is obtained by numerical minimization of the energy error expressions (which is, of course, much cheaper than numerical optimization of the Rayleigh-Ritz calculation). The asymptotic approximation to $\alpha_{\rm opt}(K)$ is remarkably good; even for K as small as 2, the relative error in the asymptotic approximation given by Eqs. (4.17)–(4.21) is 0.22% or less.

A careful examination of the exact values of $\alpha_{\rm opt}(K)$ given in the table shows that the values for $K = 2k$ agree with the values for $K = 2k + 1$ to at least ten digits. The author believes that this agreement, which holds to all digits shown for $K \leq 9$, is exact and that the disagreements beyond the tenth digit for $50 \leq K \leq 59$ are due to roundoff error in the numerical computations. A corresponding result holds for the energy error (not shown). Asymptotic methods such as those used in the present paper are not capable of proving exact results of this kind. However, the energy formula (4.12)–(4.15) can be used to show that

$$\begin{aligned}\tilde{E}^{(\mathrm{RR};K+1)} - \tilde{E}^{(\mathrm{RR};K)} &= -16\exp\left\{-\left[2\pi(4K+5)\right]^{1/2}\right\}\Bigg(\left[1+(-1)^{K+1}\right] \\ &\quad\times\left\{1+\tfrac{1}{2}\left[-\tfrac{1}{4}\ln^2\left(\frac{4K+5}{2\pi}\right)+\ln\left(\frac{4K+5}{2\pi}\right)-4\pi-\tfrac{1}{3}\pi^2\right]\right. \\ &\quad\left.\times\left[2\pi(4K+5)\right]^{-1/2}\right\}+O\left(K^{-1}\right)\Bigg). \end{aligned} \tag{4.25}$$

TABLE II. The optimum value of α, the relative errors $\delta\alpha_1/\alpha$ and $\delta\alpha_2/\alpha$ defined following Eq. (4.24) of the text, and the relative errors in the corresponding approximations to the energy error for the $\cosh^{-2}$ potential.

K	Optimum α	$\delta\alpha_1/\alpha$	$\delta\alpha_2/\alpha$	$\delta^2E_1/\delta E_R$	$\delta^2E_2/\delta E_R$
0	0.837252057937493	-2.9×10^{-2}	-3.3×10^{-3}	-4.3×10^{-1}	-1.3×10^{-1}
1	0.837252057937493	3.4×10^{-3}	-3.4×10^{-3}	-4.6×10^{-2}	-3.8×10^{-2}
2	0.852757998311315	-2.2×10^{-3}	-1.1×10^{-3}	-5.5×10^{-2}	-2.1×10^{-2}
3	0.852757998311315	2.2×10^{-3}	-8.3×10^{-4}	-3.0×10^{-2}	-2.2×10^{-2}
4	0.855289705119636	-5.5×10^{-4}	-4.9×10^{-4}	-2.3×10^{-2}	-8.5×10^{-3}
5	0.855289705119636	1.3×10^{-3}	-3.6×10^{-4}	-2.0×10^{-2}	-1.3×10^{-2}
6	0.855298109168369	-2.3×10^{-4}	-2.7×10^{-4}	-1.3×10^{-2}	-4.7×10^{-3}
7	0.855298109168369	8.7×10^{-4}	-2.1×10^{-4}	-1.5×10^{-2}	-9.0×10^{-3}
8	0.854566874022389	-1.3×10^{-4}	-1.8×10^{-4}	-9.0×10^{-3}	-3.0×10^{-3}
9	0.854566874022389	6.2×10^{-4}	-1.4×10^{-4}	-1.2×10^{-2}	-6.6×10^{-3}
10	0.853598272060356	-8.9×10^{-5}	-1.2×10^{-4}	-6.7×10^{-3}	-2.1×10^{-3}
20	0.848754323532457	-3.6×10^{-5}	-3.9×10^{-5}	-2.8×10^{-3}	-7.3×10^{-4}
30	0.845032059260072	-2.3×10^{-5}	-1.9×10^{-5}	-1.7×10^{-3}	-4.1×10^{-4}
40	0.842181310169980	-1.7×10^{-5}	-1.2×10^{-5}	-1.2×10^{-3}	-2.7×10^{-4}
50	0.839911866923864	-1.3×10^{-5}	-7.8×10^{-6}	-8.8×10^{-4}	-2.0×10^{-4}
51	0.839911866913568	4.0×10^{-5}	-7.4×10^{-6}	-2.0×10^{-3}	-6.4×10^{-4}
52	0.839510617429043	-1.2×10^{-5}	-7.3×10^{-6}	-8.4×10^{-4}	-1.9×10^{-4}
53	0.839510617417692	3.7×10^{-5}	-7.0×10^{-6}	-1.9×10^{-3}	-6.1×10^{-4}
54	0.839124247255317	-1.2×10^{-5}	-6.8×10^{-6}	-8.0×10^{-4}	-1.9×10^{-4}
55	0.839124247264764	3.5×10^{-5}	-6.5×10^{-6}	-1.9×10^{-3}	-5.8×10^{-4}
56	0.838751814909509	-1.1×10^{-5}	-6.4×10^{-6}	-7.7×10^{-4}	-1.8×10^{-4}
57	0.838751814874956	3.3×10^{-5}	-6.1×10^{-6}	-1.8×10^{-3}	-5.5×10^{-4}
58	0.838392460232471	-1.1×10^{-5}	-6.0×10^{-6}	-7.3×10^{-4}	-1.7×10^{-4}
59	0.838392460232468	3.1×10^{-5}	-5.8×10^{-6}	-1.7×10^{-3}	-5.2×10^{-4}
60	0.838045395960026	-1.1×10^{-5}	-5.7×10^{-6}	-7.0×10^{-4}	-1.6×10^{-4}

Since the factor $1+(-1)^{K+1}$ is zero for $K = 2k$, (4.25) is consistent with the empirical observation that the values for $K = 2k$ agree with the values for $K = 2k+1$, but does not prove that this agreement holds exactly. This even-odd alternation has also been observed by Klopper and Kutzelnigg [8] and can be seen in their Figs. 1–3.

The behavior in the neighborhood of $\alpha = \alpha_{\rm opt}(K)$ is obtained by Taylor expanding about $\alpha = \alpha_{\rm opt}(K)$; the result is

$$\tilde{E}^{(\mathrm{RR};K)} - E = \left[\tilde{E}^{(\mathrm{RR};K)} - E\right]_{\alpha=\alpha_{\rm opt}(K)} \times\{1 + C\left[\alpha - \alpha_{\rm opt}(K)\right]^2 + O(\left[\alpha - \alpha_{\rm opt}(K)\right]^3)\}, \tag{4.26}$$

where

$$C = \tfrac{1}{2}\pi^2(4K+5)\left[1+O\left(K^{-1/2}\right)\right]. \tag{4.27}$$

Formulas (4.26) and (4.27) show that, for K large, the minimum of $\tilde{E}^{(\mathrm{RR};K)} - E$ as a function of α is very broad on the scale set by E (because $\tilde{E}^{(\mathrm{RR};K)} - E$ is very small), but is sharp on the scale set by $\tilde{E}^{(\mathrm{RR};K)} - E$ itself.

V. THE HYDROGEN ATOM

The Hamiltonian (1.9) for the S states of the hydrogen atom (when a factor of x from the volume element is included in the wave function) has been chosen as the second example because of the physical importance of the Coulomb potential. The well known exact energies E_n and wave functions $\psi_n(x)$ for this Hamiltonian are

$$E_n = -\frac{1}{2n^2} \tag{5.1}$$

and

$$\psi_n(x) = 2n^{-5/2}x\exp(-x/n)\,L^{(1)}_{n-1}(2x/n), \tag{5.2}$$

where n is the principal quantum number. The $L^{(1)}_{n-1}$ that appears in (5.2) is a generalized Laguerre polynomial as defined in the Bateman project (see [11], pp. 188–192) and in Magnus, Oberhettinger, and Soni (see [12], pp. 239–249). This generalized Laguerre polynomial differs from the "associated Laguerre function" for which the symbol L^α_n is often used in the physics literature. The relation between the two is $[L^\alpha_n(z)]_{\rm physics} = (-1)^{n+\alpha}n!L^{(\alpha)}_{n-\alpha}(z)$. We have chosen to use this definition, which is standard in the mathematics literature, in order to facilitate the use of other relevant results from the mathematics literature. The rate of convergence of Rayleigh-Ritz approximations to the energies (5.1) will be analyzed for a variational trial function of the form

$$\tilde{\psi}_n^{(\mathrm{RR};K)}(x) = \sum_{k=0}^{K}\tilde{c}_k^{(\mathrm{RR};K)}\sqrt{2}e_{2k+1}(\alpha;x). \tag{5.3}$$

The factor $\sqrt{2}$ on the right-hand side of (5.3) appears because x is now restricted to $[0,\infty)$ while the basis functions $e_{2k+1}(\alpha;x)$ are normalized for $(-\infty,\infty)$. The exact expansion coefficients c_k to which the $\tilde{c}_k^{(\mathrm{RR};K)}$ converge as $K\to\infty$ are given by

$$c_k = \sqrt{2}\int_0^\infty e_{2k+1}(\alpha;x)\,\psi_n(x)\,dx. \tag{5.4}$$

The $k\to\infty$ asymptotic behavior of c_k will be extracted by using (3.5) to rewrite (5.4) in the form

$$c_k = c_k^{(1)} + c_k^{(2)} + c_k^{(3)}, \tag{5.5}$$

where

$$c_k^{(1)} = \sqrt{2}\int_0^{x^{(0)}_{2k+1}} e^{(+)}_{2k+1}(\alpha;x)\,\psi_n(x)\,dx, \tag{5.6}$$

$$c_k^{(2)} = \sqrt{2}\int_0^{x^{(0)}_{2k+1}} e^{(-)}_{2k+1}(\alpha;x)\,\psi_n(x)\,dx, \tag{5.7}$$

$$c_k^{(3)} = \sqrt{2}\int_{x^{(0)}_{2k+1}}^{\infty} e_{2k+1}(\alpha;x)\,\psi_n(x)\,dx. \tag{5.8}$$

The integration contours are deformed as shown in Fig. 2. Because $e^{(+)}_{2k+1}(\alpha;z)$ decays exponentially to zero as z moves off to infinity in the upper half of the complex z plane, it is convenient to deform the integration contour in (5.6) into the upper half plane. Similarly, the exponential decay of $e^{(-)}_{2k+1}(\alpha;z)$ as z tends to infinity in the lower half plane makes it convenient to deform the integration contour in (5.7) into the lower half plane. The integration contour for $c_k^{(1)}$ is pulled into the upper half plane to obtain a piece from 0 to $+i\infty$, plus a piece from $+i\infty$ to $x^{(0)}_{2k+1}$. The integration contour for $c_k^{(2)}$ is pulled into the lower half plane to obtain a piece from 0 to $-i\infty$, plus a piece from $-i\infty$ to $x^{(0)}_{2k+1}$. These contour deformations are justified by Cauchy's theorem, the exponential falloff of the $e^{(\pm)}_{2k+1}(\alpha;z)$, and the fact that the integrand has no singularities in the finite complex plane. The contributions from the pieces which run from 0 to $\pm i\infty$ are combined to give the term $c_k^{(\mathrm{cusp})}$, which comes from the cusp of the wave function at the origin. The contributions from the contours that run from $\pm i\infty$ to $x^{(0)}_{2k+1}$ are combined with $c_k^{(3)}$ to give a turning point contribution $c_k^{(\mathrm{TP})}$ of the form (3.21). The cusp contribution $c_k^{(\mathrm{cusp})}$

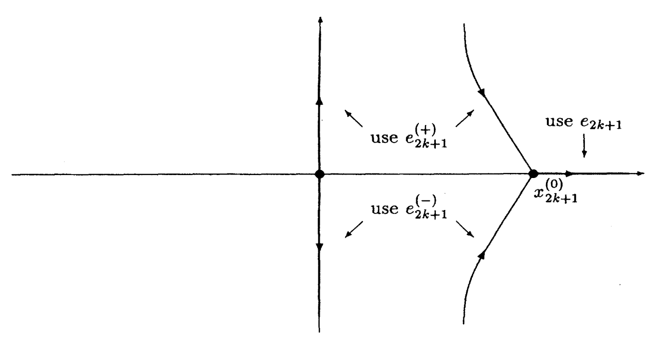

FIG. 2. Integration contours for the Coulomb potential.

can be evaluated with the aid of the asymptotic expansion (3.8). The result is

$$c_k^{(\text{cusp})} = 8\pi^{-1/2} n^{-3/2} \alpha^{-5/2} (-1)^k (4k+3)^{-7/4} \times \left[1 - \tfrac{2}{3}\left(1 + 2n^{-2}\right) \alpha^{-2} (4k+3)^{-1} + O\left(k^{-2}\right)\right]. \quad (5.9)$$

The turning point contribution can be evaluated with the aid of (3.23). The result is

$$c_k^{(\text{TP})} = 2^{1/2} \alpha^{-1/2} (4k+3)^{-1/4} \Big\{ \psi_n^{(0)}\left(x_{2k+1}^{(0)}\right) + \tfrac{1}{6}\alpha^{-3} \psi_n^{(3)}\left(x_{2k+1}^{(0)}\right) (4k+3)^{-1/2} - \left[\tfrac{1}{4}\alpha^{-2}\psi_n^{(2)}\left(x_{2k+1}^{(0)}\right) - \tfrac{1}{72}\alpha^{-6}\psi_n^{(6)}\left(x_{2k+1}^{(0)}\right)\right] \times (4k+3)^{-1} + O\left(K^{-3/2}\right) \Big\}, \quad (5.10)$$

where the superscript (j) is used to denote differentiation:

$$\psi_n^{(j)}(x) = \left(\frac{d}{dx}\right)^j \psi_n(x). \quad (5.11)$$

The desired large K asymptotic approximation to $\tilde{E}_n^{(\text{RR};K)} - E_n$ is obtained from (2.32). The result has the form

$$\tilde{E}^{(\text{RR};K)} - E = \tilde{E}_K^{(\text{cusp})} + \tilde{E}_K^{(\text{TP})} + (-1)^{K+1} \tilde{E}_K^{(\text{cross})}, \quad (5.12)$$

where $\tilde{E}_K^{(\text{cusp})}$ is the cusp contribution from (5.9), $\tilde{E}_K^{(\text{TP})}$ is the turning point contribution from (5.10), and $(-1)^{K+1} \tilde{E}_K^{(\text{cross})}$ is the cross term between the cusp and turning point contributions. The alternating sign $(-1)^{K+1}$ that appears in the cross term arises because the $c_k^{(\text{cusp})}$ alternate in sign due to the factor $(-1)^k$ in (5.9) while the $c_k^{(\text{TP})}$ are all positive. This alternating sign in the cross term is an interference effect between the cusp and the turning point contributions. The explicit formulas for these three contributions are

TABLE III. The exact error δE_R and the relative error $(\delta E_R - \delta E_A)/\delta E_R = \delta^2 E/\delta E_R$ in the approximation δE_A to δE_R for the ground state of the Coulomb potential.

	$\alpha = 1.1$		$\alpha = 1.7$		$\alpha = 2.3$	
K	δE_R	$\delta^2 E/\delta E_R$	δE_R	$\delta^2 E/\delta E_R$	δE_R	$\delta^2 E/\delta E_R$
0	1.7×10^{-1}	4.6×10^{-1}	7.5×10^{-1}	8.5×10^{-1}	1.9	1.0
1	1.3×10^{-1}	2.1×10^{-1}	4.7×10^{-1}	6.7×10^{-1}	1.1	9.1×10^{-1}
2	4.0×10^{-2}	1.4×10^{-1}	2.2×10^{-1}	5.1×10^{-1}	6.4×10^{-1}	8.1×10^{-1}
3	3.6×10^{-2}	5.0×10^{-2}	1.6×10^{-1}	3.9×10^{-1}	4.7×10^{-1}	7.1×10^{-1}
4	1.5×10^{-2}	4.7×10^{-2}	9.8×10^{-2}	3.0×10^{-1}	3.2×10^{-1}	6.1×10^{-1}
5	1.5×10^{-2}	6.2×10^{-3}	7.6×10^{-2}	2.3×10^{-1}	2.5×10^{-1}	5.3×10^{-1}
6	7.9×10^{-3}	1.6×10^{-2}	5.0×10^{-2}	1.7×10^{-1}	1.9×10^{-1}	4.6×10^{-1}
7	7.8×10^{-3}	-5.4×10^{-3}	4.0×10^{-2}	1.3×10^{-1}	1.5×10^{-1}	4.0×10^{-1}
8	4.9×10^{-3}	3.7×10^{-3}	2.7×10^{-2}	9.7×10^{-2}	1.2×10^{-1}	3.4×10^{-1}
9	4.9×10^{-3}	-8.0×10^{-3}	2.3×10^{-2}	7.3×10^{-2}	9.7×10^{-2}	3.0×10^{-1}
10	3.5×10^{-3}	-1.9×10^{-3}	1.6×10^{-2}	5.3×10^{-2}	7.8×10^{-2}	2.5×10^{-1}
20	1.4×10^{-3}	-5.3×10^{-3}	2.0×10^{-3}	-5.3×10^{-3}	1.5×10^{-2}	5.1×10^{-2}
30	8.1×10^{-4}	-4.0×10^{-3}	4.6×10^{-4}	-5.1×10^{-3}	4.2×10^{-3}	1.8×10^{-3}
40	5.4×10^{-4}	-3.2×10^{-3}	2.0×10^{-4}	-2.3×10^{-3}	1.4×10^{-3}	-9.5×10^{-3}
50	4.0×10^{-4}	-2.6×10^{-3}	1.2×10^{-4}	-1.2×10^{-3}	5.1×10^{-4}	-1.1×10^{-2}
60	3.1×10^{-4}	-2.2×10^{-3}	8.7×10^{-5}	-8.7×10^{-4}	2.1×10^{-4}	-8.9×10^{-3}
70	2.5×10^{-4}	-1.9×10^{-3}	6.9×10^{-5}	-7.2×10^{-4}	1.0×10^{-4}	-6.7×10^{-3}
80	2.0×10^{-4}	-1.7×10^{-3}	5.7×10^{-5}	-6.4×10^{-4}	5.4×10^{-5}	-4.6×10^{-3}
90	1.7×10^{-4}	-1.5×10^{-3}	4.8×10^{-5}	-5.7×10^{-4}	3.3×10^{-5}	-2.9×10^{-3}
91	1.7×10^{-4}	-1.5×10^{-3}	4.7×10^{-5}	-5.8×10^{-4}	3.3×10^{-5}	-3.1×10^{-3}
92	1.7×10^{-4}	-1.5×10^{-3}	4.6×10^{-5}	-5.6×10^{-4}	3.0×10^{-5}	-2.7×10^{-3}
93	1.6×10^{-4}	-1.5×10^{-3}	4.5×10^{-5}	-5.7×10^{-4}	3.0×10^{-5}	-2.8×10^{-3}
94	1.6×10^{-4}	-1.5×10^{-3}	4.5×10^{-5}	-5.5×10^{-4}	2.8×10^{-5}	-2.4×10^{-3}
95	1.6×10^{-4}	-1.4×10^{-3}	4.4×10^{-5}	-5.6×10^{-4}	2.8×10^{-5}	-2.6×10^{-3}
96	1.6×10^{-4}	-1.4×10^{-3}	4.3×10^{-5}	-5.4×10^{-4}	2.6×10^{-5}	-2.2×10^{-3}
97	1.5×10^{-4}	-1.4×10^{-3}	4.3×10^{-5}	-5.4×10^{-4}	2.6×10^{-5}	-2.3×10^{-3}
98	1.5×10^{-4}	-1.4×10^{-3}	4.2×10^{-5}	-5.3×10^{-4}	2.4×10^{-5}	-2.0×10^{-3}
99	1.5×10^{-4}	-1.4×10^{-3}	4.1×10^{-5}	-5.3×10^{-4}	2.4×10^{-5}	-2.1×10^{-3}
100	1.5×10^{-4}	-1.4×10^{-3}	4.1×10^{-5}	-5.2×10^{-4}	2.3×10^{-5}	-1.8×10^{-3}

$$\tilde{E}_K^{(\mathrm{cusp})} = \tfrac{16}{3}\pi^{-1}(n\alpha)^{-3}(4K+7)^{-3/2}\left\{1 - 3(\pi\alpha)^{-1}(4K+7)^{-1/2} - \left[\tfrac{4}{5}\alpha^{-2} + (n\alpha)^{-2}\right](4K+7)^{-1} + O\left(K^{-3/2}\right)\right\}, \tag{5.13}$$

$$\begin{aligned}
\tilde{E}_K^{(\mathrm{TP})} = {} & \tfrac{1}{2}\alpha^2 \int_{x_{2K+3}^{(0)}}^{\infty} \left[\phi_n^{(0)}(x)\right]^2 dx - \tfrac{1}{6}\alpha^{-1}\left\{\phi_n^{(0)}\left(x_{2K+3}^{(0)}\right)\phi_n^{(2)}\left(x_{2K+3}^{(0)}\right) - \tfrac{1}{2}\left[\phi_n^{(1)}\left(x_{2K+3}^{(0)}\right)\right]^2\right\}(4K+7)^{-1/2} \\
& - n\alpha\left[1 + \tfrac{1}{2}n\alpha(4K+7)^{-1/2}\right]\int_{x_{2K+3}^{(0)}}^{\infty} x^{-1}\phi_n^{(0)}(x)\,\psi_n(x)\,dx \\
& + \left\{\left(\tfrac{1}{4}n^{-1} - \tfrac{1}{6}\right)\left[\phi_n^{(0)}\left(x_{2K+3}^{(0)}\right)\right]^2 + \tfrac{1}{4}\phi_n^{(0)}\left(x_{2K+3}^{(0)}\right)\phi_n^{(1)}\left(x_{2K+3}^{(0)}\right)\right. \\
& - \tfrac{1}{72}\alpha^{-4}\left[\phi_n^{(0)}\left(x_{2K+3}^{(0)}\right)\phi_n^{(5)}\left(x_{2K+3}^{(0)}\right) - \phi_n^{(1)}\left(x_{2K+3}^{(0)}\right)\phi_n^{(4)}\left(x_{2K+3}^{(0)}\right) + \phi_n^{(2)}\left(x_{2K+3}^{(0)}\right)\phi_n^{(3)}\left(x_{2K+3}^{(0)}\right)\right] \\
& + \tfrac{1}{6}\left[\alpha^{-2}(n\alpha)\phi_n^{(2)}\left(x_{2K+3}^{(0)}\right) - \alpha^{-1}\phi_n^{(1)}\left(x_{2K+3}^{(0)}\right) + (n\alpha)^{-1}\phi_n^{(0)}\left(x_{2K+3}^{(0)}\right)\right] \\
& \left.\times\psi_n\left(x_{2K+3}^{(0)}\right)\right\}(4K+7)^{-1} + O\left\{K^{-3/2}\left[\phi_n^{(0)}\left(x_{2K+3}^{(0)}\right)\right]^2\right\},
\end{aligned} \tag{5.14}$$

TABLE IV. The exact error δE_R and the relative error $(\delta E_R - \delta E_A)/\delta E_R = \delta^2 E/\delta E_R$ in the approximation δE_A to δE_R for the first excited state of the Coulomb potential.

	$\alpha = 0.5$		$\alpha = 0.75$		$\alpha = 1.0$	
K	δE_R	$\delta^2 E/\delta E_R$	δE_R	$\delta^2 E/\delta E_R$	δE_R	$\delta^2 E/\delta E_R$
1	1.1×10^{-1}	7.9×10^{-1}	4.0×10^{-1}	1.0	9.5×10^{-1}	1.0
2	9.1×10^{-2}	6.1×10^{-1}	3.1×10^{-1}	9.8×10^{-1}	7.0×10^{-1}	1.1
3	3.5×10^{-2}	4.2×10^{-1}	1.6×10^{-1}	8.9×10^{-1}	4.2×10^{-1}	1.0
4	3.1×10^{-2}	3.0×10^{-1}	1.3×10^{-1}	8.0×10^{-1}	3.3×10^{-1}	1.0
5	1.5×10^{-2}	2.1×10^{-1}	7.8×10^{-2}	6.9×10^{-1}	2.3×10^{-1}	9.9×10^{-1}
6	1.4×10^{-2}	1.4×10^{-1}	6.6×10^{-2}	6.0×10^{-1}	1.9×10^{-1}	9.4×10^{-1}
7	8.2×10^{-3}	1.1×10^{-1}	4.4×10^{-2}	5.0×10^{-1}	1.5×10^{-1}	8.9×10^{-1}
8	8.0×10^{-3}	6.0×10^{-2}	3.8×10^{-2}	4.3×10^{-1}	1.2×10^{-1}	8.3×10^{-1}
9	5.1×10^{-3}	5.5×10^{-2}	2.7×10^{-2}	3.5×10^{-1}	9.7×10^{-2}	7.7×10^{-1}
10	5.1×10^{-3}	2.3×10^{-2}	2.3×10^{-2}	2.9×10^{-1}	8.4×10^{-2}	7.2×10^{-1}
20	1.6×10^{-3}	-1.8×10^{-2}	3.4×10^{-3}	1.5×10^{-2}	1.9×10^{-2}	2.6×10^{-1}
30	9.4×10^{-4}	-1.8×10^{-2}	8.4×10^{-4}	-1.8×10^{-2}	5.9×10^{-3}	6.2×10^{-2}
40	6.4×10^{-4}	-1.5×10^{-2}	3.2×10^{-4}	-1.3×10^{-2}	2.1×10^{-3}	-9.1×10^{-3}
50	4.8×10^{-4}	-1.3×10^{-2}	1.8×10^{-4}	-8.2×10^{-3}	8.4×10^{-4}	-2.9×10^{-2}
60	3.7×10^{-4}	-1.2×10^{-2}	1.3×10^{-4}	-6.0×10^{-3}	3.6×10^{-4}	-3.0×10^{-2}
70	3.0×10^{-4}	-1.0×10^{-2}	9.7×10^{-5}	-5.0×10^{-3}	1.7×10^{-4}	-2.5×10^{-2}
80	2.5×10^{-4}	-9.1×10^{-3}	7.9×10^{-5}	-4.3×10^{-3}	9.1×10^{-5}	-1.8×10^{-2}
90	2.1×10^{-4}	-8.2×10^{-3}	6.6×10^{-5}	-3.8×10^{-3}	5.4×10^{-5}	-1.2×10^{-2}
91	2.1×10^{-4}	-8.2×10^{-3}	6.5×10^{-5}	-3.7×10^{-3}	5.0×10^{-5}	-1.1×10^{-2}
92	2.1×10^{-4}	-8.1×10^{-3}	6.4×10^{-5}	-3.7×10^{-3}	4.9×10^{-5}	-1.1×10^{-2}
93	2.0×10^{-4}	-8.0×10^{-3}	6.3×10^{-5}	-3.6×10^{-3}	4.6×10^{-5}	-1.0×10^{-2}
94	2.0×10^{-4}	-7.9×10^{-3}	6.2×10^{-5}	-3.6×10^{-3}	4.6×10^{-5}	-1.0×10^{-2}
95	2.0×10^{-4}	-7.9×10^{-3}	6.1×10^{-5}	-3.6×10^{-3}	4.2×10^{-5}	-9.4×10^{-3}
96	1.9×10^{-4}	-7.8×10^{-3}	6.1×10^{-5}	-3.6×10^{-3}	4.2×10^{-5}	-9.6×10^{-3}
97	1.9×10^{-4}	-7.7×10^{-3}	5.9×10^{-5}	-3.5×10^{-3}	3.9×10^{-5}	-8.5×10^{-3}
98	1.9×10^{-4}	-7.6×10^{-3}	5.9×10^{-5}	-3.5×10^{-3}	3.9×10^{-5}	-8.8×10^{-3}
99	1.9×10^{-4}	-7.6×10^{-3}	5.8×10^{-5}	-3.4×10^{-3}	3.6×10^{-5}	-7.8×10^{-3}
100	1.8×10^{-4}	-7.5×10^{-3}	5.7×10^{-5}	-3.4×10^{-3}	3.6×10^{-5}	-8.0×10^{-3}

$$\tilde{E}_K^{(\text{cross})} = 4\left(\frac{2\alpha}{\pi}\right)^{1/2} (n\alpha)^{-3/2} (-1)^{K+1} (4K+7)^{-3/2} \left\{ \phi_n^{(0)}\left(x_{2K+3}^{(0)}\right) + \left[\tfrac{1}{6}\alpha^{-3}\phi_n^{(3)}\left(x_{2K+3}^{(0)}\right) - n\psi_n\left(x_{2K+3}^{(0)}\right) - \left(\frac{2}{\pi\alpha}\right)\phi_n^{(0)}\left(x_{2K+3}^{(0)}\right)\right] \times (4K+7)^{-1/2} + O\left[K^{-1}\phi_n^{(0)}\left(x_{2K+3}^{(0)}\right)\right] \right\}, \tag{5.15}$$

where

$$\phi_n^{(j)}(x) = \left(\frac{d}{dx}\right)^j \left[(n\alpha)^{-1}\psi_n^{(0)}(x) - \alpha^{-1}\psi_n^{(1)}(x)\right] = \left(\frac{d}{dx}\right)^j [-2n^{-3/2}\alpha^{-1} \times \exp(-x/n)\, L_n^{(0)}(2x/n)] \, . \tag{5.16}$$

Tables III and IV compare the exact values of the error $\delta E_R = \tilde{E}^{(\text{RR};K)} - E$ obtained by performing the Rayleigh-Ritz calculation with the asymptotic approximation δE_A to δE_R given by the right-hand side of (5.12) when the terms are given by (5.13)–(5.15). The tables list the relative error $\delta^2 E/\delta E_R = (\delta E_R - \delta E_A)/\delta E_R$ for three different values of α for the ground and the first excited states. The relation of the values of α for which

TABLE V. The optimum value of α, the relative error $\delta\alpha/\alpha$ in the asymptotic approximation to optimum α, the exact energy error δE_R, and the relative error $(\delta E_R - \delta E_A)/\delta E_R = \delta^2 E/\delta E_R$ in the approximation δE_A to δE_R when α has its optimum value for the Coulomb potential ground state.

K	Optimum α	$\delta\alpha/\alpha$	δE_R	$\delta^2 E/\delta E_R$
0	0.752252778063675		$7.55868184216124\times10^{-2}$	
1	0.752252778063675		$7.55868184216124\times10^{-2}$	
2	0.896347159407260	1.0×10^{-2}	$2.73603230438885\times10^{-2}$	1.3×10^{-1}
3	0.896347159407260	3.4×10^{-3}	$2.73603230438885\times10^{-2}$	1.2×10^{-2}
4	0.987049713223452	-4.0×10^{-3}	$1.33923293865637\times10^{-2}$	3.7×10^{-2}
5	0.987049713223452	-3.3×10^{-3}	$1.33923293865637\times10^{-2}$	-4.5×10^{-3}
6	1.05777265075453	-3.4×10^{-3}	$7.70858429223468\times10^{-3}$	1.3×10^{-2}
7	1.05777265075453	-2.4×10^{-3}	$7.70858429223468\times10^{-3}$	-7.3×10^{-3}
8	1.11766782540575	-2.3×10^{-3}	$4.91074973109288\times10^{-3}$	4.8×10^{-3}
9	1.11766782540575	-1.5×10^{-3}	$4.91074973109288\times10^{-3}$	-7.5×10^{-3}
10	1.17053329225231	-1.5×10^{-3}	$3.35386955983412\times10^{-3}$	1.0×10^{-3}
20	1.37759400674291	2.3×10^{-5}	$8.81057671750606\times10^{-4}$	-2.4×10^{-3}
30	1.53481298788369	3.1×10^{-4}	$3.69588376089098\times10^{-4}$	-2.2×10^{-3}
40	1.66565123809335	3.7×10^{-4}	$1.93654849090432\times10^{-4}$	-1.9×10^{-3}
50	1.77949989362499	3.8×10^{-4}	$1.15646688461433\times10^{-4}$	-1.6×10^{-3}
60	1.88126421247228	3.7×10^{-4}	$7.52877574735171\times10^{-5}$	-1.4×10^{-3}
70	1.97388709435364	3.6×10^{-4}	$5.21129367805738\times10^{-5}$	-1.3×10^{-3}
80	2.05929577974590	3.4×10^{-4}	$3.77638940367880\times10^{-5}$	-1.2×10^{-3}
90	2.13883191608814	3.2×10^{-4}	$2.83573402211951\times10^{-5}$	-1.1×10^{-3}
91	2.13883191608814	3.5×10^{-4}	$2.83573402211951\times10^{-5}$	-1.2×10^{-3}
92	2.15412524298853	3.2×10^{-4}	$2.68749528892947\times10^{-5}$	-1.1×10^{-3}
93	2.15412524298854	3.5×10^{-4}	$2.68749528892947\times10^{-5}$	-1.2×10^{-3}
94	2.16923000202692	3.2×10^{-4}	$2.54977199604414\times10^{-5}$	-1.0×10^{-3}
95	2.16923000202691	3.5×10^{-4}	$2.54977199604414\times10^{-5}$	-1.2×10^{-3}
96	2.18415234251192	3.2×10^{-4}	$2.42162860538889\times10^{-5}$	-1.0×10^{-3}
97	2.18415234251194	3.4×10^{-4}	$2.42162860538889\times10^{-5}$	-1.2×10^{-3}
98	2.19889809378137	3.1×10^{-4}	$2.30222908966460\times10^{-5}$	-1.0×10^{-3}
99	2.19889809378137	3.4×10^{-4}	$2.30222908966460\times10^{-5}$	-1.2×10^{-3}
100	2.21347278783437	3.1×10^{-4}	$2.19082467767284\times10^{-5}$	-1.0×10^{-3}

the error is tabulated in Tables III and IV to the optimum value of α for specific values of K can be determined from Tables V and VI. A comparison of Tables III and IV shows that the asymptotic approximation (5.12)–(5.16) is not as good for the first excited state as it is for the ground state. The corresponding results for the second and the third excited states (not shown) exhibit a further deterioration in the accuracy of the asymptotic approximation (5.12)–(5.16). This deterioration is to be expected. Excited states are more spread out than the ground state and α is smaller, which implies that the asymptotic expansion (3.8), which was used in the derivation of the asymptotic approximation (5.9) to $c_k^{(\mathrm{cusp})}$, is less accurate. This could presumably be fixed by using instead the more complicated expansion (3.10). Furthermore, excited states wiggle more, which implies that the asymptotic approximation (5.10) to $c_k^{(\mathrm{TP})}$, which was obtained from (3.23), is less accurate. A more sophisticated asymptotic analysis could presumably be worked out to cope with this difficulty also. However, such extensions go well beyond the intended purpose of the present paper and have therefore not been attempted.

The asymptotic approximation (5.12)–(5.16) for the error can be optimized with respect to the nonlinear parameter α to obtain an asymptotic approximation to the value $\alpha_{\mathrm{opt}}(K)$ that yields the best approximation to the energy for a given value of K. To lowest order for large K, $\alpha_{\mathrm{opt}}(K) \approx \alpha_{\mathrm{opt}}^{(0)}(K)$, where

$$\alpha_{\mathrm{opt}}^{(0)}(K) = \frac{2(4K+7)^{1/2}}{ny^{(0)}}, \qquad (5.17)$$

with $y^{(0)}$ the largest root of

$$\exp\left(-y^{(0)}\right)\left[\frac{L_n^{(0)}\left(y^{(0)}\right)}{y^{(0)}}\right]^2 = \frac{2n^2}{\pi(4K+7)^3}. \qquad (5.18)$$

The result (5.17) and (5.18) is obtained by keeping only the leading terms in $\tilde{E}_K^{(\mathrm{cusp})}$ and $\tilde{E}_K^{(\mathrm{TP})}$ and neglecting $(-1)^{K+1}\tilde{E}_K^{(\mathrm{cross})}$. Since the root $y^{(0)}$ must be computed via numerical methods, no attempt has been made to compute higher-order analytic formulas for $\alpha_{\mathrm{opt}}(K)$; the higher-order results are obtained via a direct numerical minimization of (5.12)–(5.15). The results of this direct numerical minimization for the ground and first excited states are presented in Tables V and VI. This minimization failed for $0 \le K \le 1$ for the ground state and failed

TABLE VI. The optimum value of α, the relative error $\delta\alpha/\alpha$ in the asymptotic approximation to optimum α, the exact energy error δE_R, and the relative error $(\delta E_R - \delta E_A)/\delta E_R = \delta^2 E/\delta E_R$ in the approximation δE_A to δE_R when α has its optimum value for the Coulomb potential first excited state.

K	Optimum α	$\delta\alpha/\alpha$	δE_R	$\delta^2 E/\delta E_R$
1	0.282860033712878		$3.75395287706990\times10^{-2}$	
2	0.282860033712878		$3.75395287706990\times10^{-2}$	
3	0.359994434593618		$1.89258369817236\times10^{-2}$	
4	0.359994434593618		$1.89258369817236\times10^{-2}$	
5	0.408317667711692		$1.11417200479054\times10^{-2}$	
6	0.408317667711692		$1.11417200479054\times10^{-2}$	
7	0.444213305336506	2.6×10^{-2}	$7.21529231314512\times10^{-3}$	1.3×10^{-1}
8	0.444213305336506	2.3×10^{-2}	$7.21529231314512\times10^{-3}$	6.5×10^{-2}
9	0.473359830848861	6.9×10^{-4}	$4.98768980888883\times10^{-3}$	5.3×10^{-2}
10	0.473359830848861	1.3×10^{-3}	$4.98768980888883\times10^{-3}$	2.1×10^{-2}
20	0.575683110461752	-1.7×10^{-3}	$1.34834750295180\times10^{-3}$	-1.3×10^{-2}
30	0.647916071569366	-1.3×10^{-5}	$5.70621173466940\times10^{-4}$	-1.2×10^{-2}
40	0.706725966058271	6.3×10^{-4}	$2.99878623258467\times10^{-4}$	-1.0×10^{-2}
50	0.757437341468158	8.9×10^{-4}	$1.79215758234553\times10^{-4}$	-8.5×10^{-3}
60	0.802564820295123	9.8×10^{-4}	$1.16647730162865\times10^{-4}$	-7.2×10^{-3}
70	0.843539526203126	1.0×10^{-3}	$8.06886175723896\times10^{-5}$	-6.2×10^{-3}
80	0.881270313303385	1.0×10^{-3}	$5.84206286912019\times10^{-5}$	-5.5×10^{-3}
90	0.916377769483651	9.9×10^{-4}	$4.38264338171239\times10^{-5}$	-4.9×10^{-3}
91	0.923125996979864	9.2×10^{-4}	$4.15271552432062\times10^{-5}$	-4.5×10^{-3}
92	0.923125996979864	9.8×10^{-4}	$4.15271552432062\times10^{-5}$	-4.8×10^{-3}
93	0.929790437979584	9.1×10^{-4}	$3.93912001388599\times10^{-5}$	-4.4×10^{-3}
94	0.929790437979584	9.8×10^{-4}	$3.93912001388599\times10^{-5}$	-4.7×10^{-3}
95	0.936373877424941	9.1×10^{-4}	$3.74040378296727\times10^{-5}$	-4.3×10^{-3}
96	0.936373877424941	9.7×10^{-4}	$3.74040378296727\times10^{-5}$	-4.6×10^{-3}
97	0.942878951401551	9.1×10^{-4}	$3.55526818272669\times10^{-5}$	-4.2×10^{-3}
98	0.942878951401551	9.7×10^{-4}	$3.55526818272669\times10^{-5}$	-4.6×10^{-3}
99	0.949308158024396	9.0×10^{-4}	$3.38254999623107\times10^{-5}$	-4.2×10^{-3}
100	0.949308158024396	9.6×10^{-4}	$3.38254999623107\times10^{-5}$	-4.5×10^{-3}

for $1 \le K \le 6$ for the first excited state; for this reason no relative errors are listed for these values of K. This failure for small values of K occurs because (5.12)–(5.15) are a large K asymptotic approximation that breaks down for small K and does not even have a minimum, when the approximation is carried to three terms. The breakdown can be cured by taking only one term. The one-term results are, of course, less accurate than those shown in Tables V and VI.

Klopper and Kutzelnigg [8] have conjectured that the error in the energy decreases like K^{-2} for large K when the variational calculation is optimized with respect to α. Equations (5.12)–(5.18) are not consistent with this conjecture, which was based on empirical curve fitting over a limited range of K.

VI. THE x^4 ANHARMONIC OSCILLATOR

The anharmonic oscillator Hamiltonian (1.10) has been chosen as the third example because its bound state wave functions are entire. Thus there are no wave function singularity contributions to compete with basis function turning point contributions in this case. The formulas (3.23) and (3.24) for basis function turning point contributions fail for this example, which illustrates a different mechanism for the determination of optimum α.

Although the Schrödinger equation for the anharmonic oscillator cannot be solved exactly in terms of known, well-studied functions, its eigenvalues can be calculated to high accuracy. For the ground state with $\lambda = 1$,

$$E = 1.392\,351\,641\,530\,291\,855\,657\,507\,9\ldots\,. \tag{6.1}$$

The value of E given in (6.1) was obtained by using variational methods [20] to calculate rigorous upper and lower bounds to E that agree to the number of digits shown. The rate of convergence of Rayleigh-Ritz approximations to the ground state energy (6.1) will be analyzed for a variational trial function of the form

$$\tilde{\psi}^{(\mathrm{RR};K)}(x) = \sum_{k=0}^{K} \tilde{c}_k^{(\mathrm{RR};K)} e_{2k}(\alpha; x)\,. \tag{6.2}$$

The exact expansion coefficients c_k to which the $\tilde{c}_k^{(\mathrm{RR};K)}$ converge as $K \to \infty$ are given by

$$c_k = \int_{-\infty}^{\infty} e_{2k}(\alpha; x)\,\psi(x)\,dx. \tag{6.3}$$

The information about the wave function $\psi(x)$ that is needed to construct a large k asymptotic approximation to the integral (6.3) can be obtained from asymptotic expansions of $\psi(z)$ that are valid for large complex z; the details are in Eqs. (C1)–(C9) of Appendix C. Equation (3.5) is used to obtain

$$c_k = c_k^{(+)} + c_k^{(-)}, \tag{6.4}$$

where

$$c_k^{(\pm)} = \int_{-\infty}^{\infty} e_{2k}^{(\pm)}(\alpha; z)\,\psi(z)\,dz. \tag{6.5}$$

The wave function $\psi(z)$ decreases like $\exp\left(-\frac{1}{3}\lambda^{1/2}|z|^3 - \frac{1}{2}\lambda^{-1/2}|z|\right)$ for large real z, which is enough to make the integrals (6.5) convergent at infinity despite the exponential growth of the $e_{2k}^{(\pm)}(\alpha; z)$ that is apparent from (3.7). Large k asymptotic approximations to the integrals (6.5) can be obtained via the saddle point method.

The saddle point method (see [21], pp. 440–443; [22], Chap. 7; or [23], pp. 84–116) of approximating an integral begins by writing the integral in the form

$$I = \int g(z)\exp[w(z)]\,dz. \tag{6.6}$$

Saddle points occur at the zeros of $w(z)$. It is assumed that $w(z)$ and $g(z)$ are analytic functions of z, that the integration contour passes through one or more saddle points, and that most of the contribution to the integral comes from neighborhoods of the saddle points. Suppose that z_0 is a saddle point that is a simple zero of $w(z)$. The saddle point method, also known as the method of steepest descent, obtains an approximation to the contribution from the neighborhood of a saddle point z_0 by evaluating $g(z)$ at z_0 and Taylor expanding $w(z)$ about the saddle point:

$$w(z) \approx w(z_0) + \tfrac{1}{2}w''(z_0)(z - z_0)^2\,. \tag{6.7}$$

The saddle point formula

$$I \approx \sqrt{\frac{2\pi}{\exp(\pm i\pi)\,w''(z_0)}}\,g(z_0)\exp[w(z_0)] \tag{6.8}$$

is obtained by inserting these approximations into (6.6), extending the path of integration to infinity on either side of the saddle point, and integrating. The approximation (6.8) can be expected to be accurate if $|w''(z_0)|$ is large, which is the condition for the integrand to have a sharp peak at the saddle point. Contributions to the integral from well separated saddle points can be computed separately and added. Rigorous justification, and analyses of a number of interesting cases in which the simple saddle point method described above breaks down, can be found in [22], Chaps. 7 and 9, and [23], pp. 84–116 and Chap. VII.

The saddle points for the integral (6.5) are at the points $\pm z_+$ and $\pm z_-$, where

$$z_+ = \frac{1}{2\lambda^{1/2}}\left(q_1 + \alpha^2\delta\right), \tag{6.9}$$

$$z_- = \frac{1}{2\lambda^{1/2}}\left(q_1 - \alpha^2\delta\right), \tag{6.10}$$

with

$$q_1 = \sqrt{\alpha^4 - 1 + q_0}\,, \tag{6.11}$$

$$\delta = \alpha^{-2}\sqrt{\alpha^4 - 1 - q_0}\,, \tag{6.12}$$

$$q_0 = \sqrt{1 + 4\lambda\alpha^2(2k+1)}\,. \tag{6.13}$$

The saddle points z_+ and z_- coalesce for $k = k_c$, where

$$k_c = -\frac{1}{2} + \frac{\alpha^6 - 2\alpha^2}{8\lambda}. \tag{6.14}$$

For $k < k_c$, z_+ and z_- are real with $z_- < z_+$. For $k > k_c$, z_+ and z_- are complex conjugates. The integration contours for the integrals (6.5) are deformed to follow paths of steepest descent through the saddle points as shown in Figs. 3 and 4. Essentially all of the contribution to the integrals for large k comes from the neighborhoods of the saddle points. The formulas for the ordinary saddle point method break down as the saddle points approach each other. The more complicated formulas for asymptotic expansions of integrals with two nearby saddle points must then be used (see [22], pp. 369–379, or [23], pp. 366–372). Since these more complicated formulas reduce to the ordinary saddle point formulas when the saddle points are not close to each other, there is no need to use the ordinary saddle point formulas at all; the formulas for two nearby saddle points will provide the needed large k expansion that is uniformly valid in α. The result has the form

$$c_k = 2\pi i \exp(\rho) \left[a_0 \mathrm{Ai}\left(\gamma^2\right) + a_1 \mathrm{Ai}'\left(\gamma^2\right)\right] \left[1 + O\left(k^{-1}\right)\right]. \tag{6.15}$$

The parameters ρ and γ and the coefficients a_0 and a_1 are given by Eqs. (C21)–(C27), (C32), and (C33) of Appendix C. The formula (6.15) for two nearby saddle points is obtained by transforming the integrand for the desired integral (approximately) into the integrand of Airy's integral; this is why the Airy function Ai and its derivative Ai$'$ appear in (6.15). The idea is similar to that used in the ordinary saddle point method, where the integrand for the desired integral is approximated by a Gaussian.

The ground state energy of the oscillator Hamiltonian $H^{(c)}$ is 1 when $\lambda = 0$ and increases as λ increases. Therefore $H^{(c)}$ is a positive definite operator. The matrix elements of $H^{(c)}$ are

$$\begin{aligned} H^{(c)}_{k,\ell} &= \int_{-\infty}^{\infty} e_{2k}(\alpha;x) \left[\left(-\frac{d^2}{dx^2} + x^2 + \lambda x^4\right) e_{2\ell}(\alpha;x)\right] dx \\ &= \tfrac{1}{4}\lambda\alpha^{-4}\left[(2\ell+4)(2\ell+3)(2\ell+2)(2\ell+1)\right]^{1/2} \delta_{k,\ell+2} \\ &\quad + \left[\tfrac{1}{2}\lambda\alpha^{-4}(4\ell+3) + \tfrac{1}{2}\alpha^{-2} - \tfrac{1}{2}\alpha^2\right]\left[(2\ell+2)(2\ell+1)\right]^{1/2} \delta_{k,\ell+1} \\ &\quad + \left[\tfrac{3}{4}\lambda\alpha^{-4}\left(8\ell^2+4\ell+1\right) + \left(\tfrac{1}{2}\alpha^{-2} + \tfrac{1}{2}\alpha^2\right)(4\ell+1)\right] \delta_{k,\ell} \\ &\quad + \left[\tfrac{1}{2}\lambda\alpha^{-4}(4\ell-1) + \tfrac{1}{2}\alpha^{-2} - \tfrac{1}{2}\alpha^2\right]\left[2\ell(2\ell-1)\right]^{1/2} \delta_{k,\ell-1} \\ &\quad + \tfrac{1}{4}\lambda\alpha^{-4}\left[2\ell(2\ell-1)(2\ell-2)(2\ell-3)\right]^{1/2} \delta_{k,\ell-2}. \end{aligned} \tag{6.16}$$

Hence it is convenient to make the choice $B = H^{(c)}$ for the positive definite operator B, which is used to construct the B-Hilbert space in the general theory developed in Sec. II. The requirement that the matrix elements $B_{k,\ell}$ of B be approximately equal to the matrix elements $H^{(c)}_{k,\ell} - E\delta_{k,\ell}$ for k and ℓ large is then obviously satisfied. The error in the Rayleigh-Ritz calculation is then given approximately by the first term in the numerator of (2.32)

$$\tilde{E}^{(\mathrm{RR};K)} - E \approx \langle \delta\psi^{(B;K)} | (H - EI) | \delta\psi^{(B;K)} \rangle = \sum_{k=K+1}^{\infty} |\hat{c}_k|^2. \tag{6.17}$$

The sum over k in (6.17) converges rapidly as a conse-

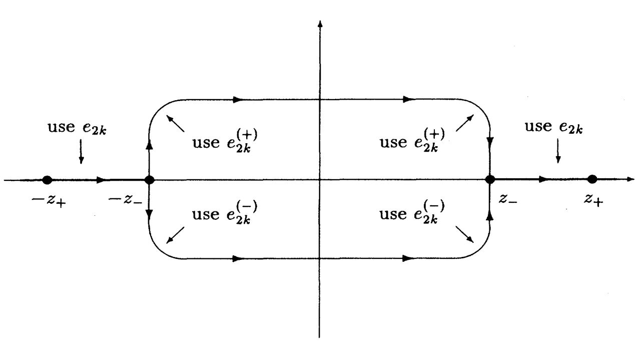

FIG. 3. Integration contours for the anharmonic oscillator when $k < k_c$.

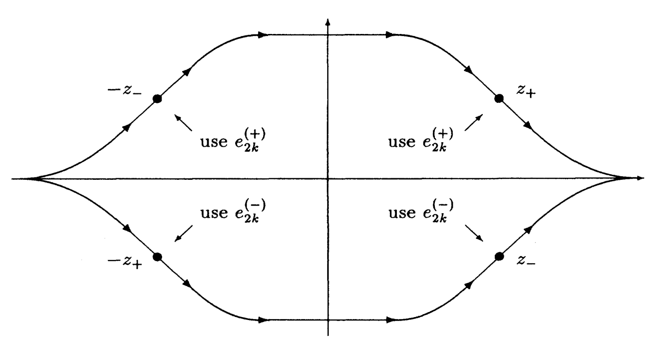

FIG. 4. Integration contours for the anharmonic oscillator when $k > k_c$.

TABLE VII. The exact error δE_R and the relative error $(\delta E_R - \delta E_A)/\delta E_R = \delta^2 E/\delta E_R$ in the approximation δE_A to δE_R for the anharmonic oscillator ground state.

	$\alpha = 1.0$		$\alpha = 2.0$		$\alpha = 3.0$	
K	δE_R	$\delta^2 E/\delta E_R$	δE_R	$\delta^2 E/\delta E_R$	δE_R	$\delta^2 E/\delta E_R$
0	3.6×10^{-1}	-1.1×10^{-2}	7.8×10^{-1}	4.7×10^{-1}	3.2	8.3×10^{-1}
1	2.0×10^{-2}	4.8×10^{-2}	1.3×10^{-1}	5.1×10^{-2}	1.2	6.8×10^{-1}
2	2.7×10^{-3}	-3.8×10^{-1}	1.5×10^{-2}	-4.7×10^{-2}	5.7×10^{-1}	4.3×10^{-1}
3	2.6×10^{-3}	-2.4×10^{-1}	8.9×10^{-4}	-5.7×10^{-2}	2.7×10^{-1}	2.4×10^{-1}
4	1.0×10^{-3}	-1.3×10^{-1}	1.9×10^{-5}	-6.4×10^{-2}	1.3×10^{-1}	1.2×10^{-1}
5	2.1×10^{-4}	-5.1×10^{-2}	3.3×10^{-8}	-1.8×10^{-2}	5.7×10^{-2}	5.6×10^{-2}
6	2.3×10^{-5}	1.8×10^{-2}	3.2×10^{-8}	-3.1×10^{-2}	2.4×10^{-2}	2.4×10^{-2}
7	3.9×10^{-6}	-1.4×10^{-1}	7.5×10^{-10}	-5.0×10^{-2}	9.6×10^{-3}	9.4×10^{-3}
8	3.8×10^{-6}	-1.4×10^{-1}	2.6×10^{-11}	-1.1×10^{-2}	3.6×10^{-3}	2.7×10^{-3}
9	2.3×10^{-6}	-8.9×10^{-2}	3.4×10^{-12}	-3.3×10^{-2}	1.3×10^{-3}	-4.7×10^{-4}
10	8.0×10^{-7}	-5.2×10^{-2}	2.3×10^{-14}	1.2×10^{-3}	4.3×10^{-4}	-2.1×10^{-3}
11	1.8×10^{-7}	-1.8×10^{-2}	1.2×10^{-14}	-2.6×10^{-2}	1.4×10^{-4}	-3.1×10^{-3}
12	2.3×10^{-8}	1.2×10^{-2}	5.2×10^{-17}	-1.0×10^{-2}	4.1×10^{-5}	-3.8×10^{-3}
13	5.5×10^{-9}	-9.2×10^{-2}	4.8×10^{-17}	-2.2×10^{-2}	1.2×10^{-5}	-4.3×10^{-3}
14	5.5×10^{-9}	-9.6×10^{-2}	2.3×10^{-19}	-1.2×10^{-2}	3.2×10^{-6}	-4.7×10^{-3}
15	3.7×10^{-9}	-6.6×10^{-2}	2.2×10^{-19}	-2.0×10^{-2}	8.3×10^{-7}	-5.0×10^{-3}
16	1.6×10^{-9}	-4.3×10^{-2}	1.6×10^{-21}	-2.2×10^{-3}	2.0×10^{-7}	-5.2×10^{-3}
17	4.9×10^{-10}	-2.2×10^{-2}	1.1×10^{-21}	-2.0×10^{-2}	4.8×10^{-8}	-5.3×10^{-3}
18	9.6×10^{-11}	7.2×10^{-4}	1.8×10^{-23}	-9.9×10^{-4}	1.1×10^{-8}	-5.4×10^{-3}
19	1.5×10^{-11}	-9.1×10^{-3}	5.7×10^{-24}	-2.0×10^{-2}	2.3×10^{-9}	-5.5×10^{-3}
20	8.1×10^{-12}	-8.1×10^{-2}	2.5×10^{-25}	-5.5×10^{-3}	4.7×10^{-10}	-5.5×10^{-3}
21	7.7×10^{-12}	-6.5×10^{-2}	2.5×10^{-26}	-2.3×10^{-2}	9.2×10^{-11}	-5.5×10^{-3}
22	4.9×10^{-12}	-4.7×10^{-2}	3.2×10^{-27}	-9.4×10^{-3}	1.7×10^{-11}	-5.5×10^{-3}
23	2.2×10^{-12}	-3.1×10^{-2}	6.9×10^{-29}	-2.8×10^{-2}	3.0×10^{-12}	-5.5×10^{-3}
24	7.0×10^{-13}	-1.7×10^{-2}	3.3×10^{-29}	-1.3×10^{-2}	5.2×10^{-13}	-5.5×10^{-3}

TABLE VIII. The optimum value of α, the relative error $\delta\alpha_1/\alpha$ in the asymptotic approximation to optimum α, the exact energy error δE_R, and the relative error $(\delta E_R - \delta E_A)/\delta E_R = \delta^2 E/\delta E_R$ in the approximation δE_A to δE_R when α has its optimum value for the anharmonic oscillator ground state.

K	Optimum α	$\delta\alpha/\alpha$	δE_R	$\delta^2 E/\delta E_R$
0	1.29294233500847	1.6×10^{-2}	$1.09716442402927\times10^{-2}$	-2.4×10^{-1}
1	1.55817459174733	3.4×10^{-3}	$4.82503172746064\times10^{-4}$	-1.1×10^{-1}
2	1.71862312909596	1.4×10^{-3}	$3.38631249912197\times10^{-5}$	-6.7×10^{-2}
3	1.57714593232280	1.4×10^{-3}	$2.60189681146471\times10^{-6}$	-7.5×10^{-2}
4	1.70670645005687	7.3×10^{-4}	$1.33517756262170\times10^{-7}$	-5.4×10^{-2}
5	1.80836293245295	4.4×10^{-4}	$8.57004518662618\times10^{-9}$	-4.2×10^{-2}
6	1.89219980394674	3.0×10^{-4}	$6.40347751665497\times10^{-10}$	-3.4×10^{-2}
7	1.80766391482629	3.1×10^{-4}	$3.87351871813567\times10^{-11}$	-3.6×10^{-2}
8	1.88374660430946	2.2×10^{-4}	$2.41714403978924\times10^{-12}$	-3.0×10^{-2}
9	1.95004181438340	1.6×10^{-4}	$1.69012176051751\times10^{-13}$	-2.6×10^{-2}
10	2.00883309590816	1.2×10^{-4}	$1.29345957264323\times10^{-14}$	-2.3×10^{-2}
11	2.06168891078903	9.9×10^{-5}	$1.06545539864153\times10^{-15}$	-2.0×10^{-2}
12	2.00233192434442	1.0×10^{-4}	$4.859841517497\times10^{-17}$	-2.1×10^{-2}
13	2.05246975581368	8.3×10^{-5}	$3.53462977274\times10^{-18}$	-1.9×10^{-2}
14	2.09841072018140	6.8×10^{-5}	$2.7410652496\times10^{-19}$	-1.7×10^{-2}
15	2.14082155033793	5.7×10^{-5}	$2.246129143\times10^{-20}$	-1.6×10^{-2}
16	2.18022179759981	4.8×10^{-5}	1.93093405×10^{-21}	-1.4×10^{-2}
17	2.13382604863630	5.0×10^{-5}	7.680461×10^{-23}	-1.5×10^{-2}
18	2.17183819567434	4.3×10^{-5}	6.00718×10^{-24}	-1.4×10^{-2}
19	2.20749144840388	3.7×10^{-5}	4.9101×10^{-25}	-1.3×10^{-2}

quence of the rapid decrease of the c_k with increasing k. Therefore no attempt has been made to deduce asymptotic formulas for the $U_{k,\ell}$ that appear in (2.19). The $U_{k,\ell}$ are obtained via numerical Cholesky decomposition of $B = H^{(c)}$ with the aid of (2.14) and (2.15). Numerical values of the $\hat{c}_k$ are then obtained by using these numerically determined $U_{k,\ell}$ and the asymptotic approximations to the c_k in (2.19). Numerical values of the sum over k in (6.17) can then be computed. The error as predicted by (6.17) is compared with the exact error in Table VII for $\lambda = 1$, $\alpha = 1$, for $\lambda = 1$, $\alpha = 2$, and for $\lambda = 1$, $\alpha = 3$. Table VIII compares the estimates for optimum α obtained by numerical minimization of (6.17) with exact values of optimum α.

Table VII shows that the error estimates obtained from (6.17) are good to 2% or better for $K > 3$ and that these error estimates improve as α increases. Table VIII shows that the approximation to optimum α obtained by numerical minimization of the error estimate (6.17) is good to better than 0.1% for $K > 3$. The values of the exact energy error δE_R given in both tables show the rapid convergence of the Rayleigh-Ritz method for this example, which is reflected in the rapid convergence of the sum over k in (6.17).

VII. OTHER BASIS SETS

The asymptotic analysis of the expansion coefficients for the basis set is the first step in deriving the convergence behavior of a Rayleigh-Ritz calculation via the methods developed in Sec. II. This section outlines two methods of performing this asymptotic analysis that the author has found useful and illustrates them with an example. The section begins by extending the method used above for Hermite polynomial basis sets to Jacobi and generalized Laguerre polynomial basis sets. A generating function method is considered next. The same Laguerre polynomial expansion is used as an example for both methods. Either method will work for all of the classical orthogonal polynomials (Gegenbauer, Legendre, and Chebyshev polynomials are special cases of Jacobi polynomials; spherical harmonics can be assembled from Gegenbauer polynomials).

The asymptotic analysis of the expansion coefficients for Hermite polynomial basis sets was carried out by using Eqs. (3.3)–(3.5) to rewrite the integrals (4.4), (5.4), and (6.3) for the expansion coefficients c_k as contour integrals. Large k asymptotic approximations to these contour integrals were then constructed by deforming the contour and using standard methods for the asymptotic analysis of integrals [22–24]. Asymptotic approximations to the Hermite basis functions and the parabolic cylinder functions were needed to implement this program. The needed asymptotic formulas for these special functions were available in the literature; no attempt was made to derive them. Similar formulas can be found for other special functions; the tools used are the Liouville-Green approximation $q^{-1/2}\exp\left(\pm i\int q dz\right)$ to the solution of the differential equation $f'' + q^2 f = 0$, which is familiar from the WKB method and can be used to derive (3.9)–(3.12), and its generalization, which is needed to derive (3.14)–(3.20). The generalization can be traced back to papers by Langer [25] in 1931 and 1932; a very readable paper of Miller and Good [26] explains the basic idea. A convenient formulation of this generalization has been given by Olver, whose book includes some historical notes (see [24], p. 433).

The extension of the approach used above for Hermite polynomials to Jacobi and generalized Laguerre polynomials starts with the expansions

$$f^{(J)}(x) = \sum_{k=0}^{\infty} c_k^{(J;\alpha,\beta)} (1-x)^{\alpha/2} (1+x)^{\beta/2} P_k^{(\alpha,\beta)}(x), \tag{7.1}$$

$$f^{(L)}(x) = \sum_{k=0}^{\infty} c_k^{(L;\alpha)} \exp(-x/2)\, x^{\alpha/2} L_k^{(\alpha)}(x). \tag{7.2}$$

The standard orthogonality argument yields the formulas

$$c_k^{(J;\alpha,\beta)} = I_k^{(J;\alpha,\beta)} / h_k^{(J;\alpha,\beta)}, \tag{7.3}$$

$$c_k^{(L;\alpha)} = I_k^{(L;\alpha)} / h_k^{(L;\alpha)} \tag{7.4}$$

for the coefficients, where

$$h_k^{(J;\alpha,\beta)} = \int_{-1}^{1} \left[P_k^{(\alpha,\beta)}(x)\right]^2 (1-x)^{\alpha} (1+x)^{\beta}\, dx = \frac{2^{\alpha+\beta+1}\Gamma(k+\alpha+1)\,\Gamma(k+\beta+1)}{(2k+\alpha+\beta+1)\, k!\,\Gamma(k+\alpha+\beta+1)}, \tag{7.5}$$

$$I_k^{(J;\alpha,\beta)} = \int_{-1}^{1} f^{(J)}(x)\, P_k^{(\alpha,\beta)}(x)\, (1-x)^{\alpha/2} \times (1+x)^{\beta/2}\, dx, \tag{7.6}$$

$$h_k^{(L;\alpha)} = \int_0^{\infty} \left[L_k^{(\alpha)}\right]^2 (x)\, x^{\alpha} \exp(-x)\, dx = \frac{\Gamma(k+\alpha+1)}{k!}, \tag{7.7}$$

$$I_k^{(L;\alpha)} = \int_0^{\infty} f^{(L)}(x)\, L_k^{(\alpha)}(x)\, x^{\alpha/2} \exp(-x/2)\, dx. \tag{7.8}$$

The analogs of Eqs. (3.3)–(3.5), which can be used to rewrite (7.6) and (7.8) as integrals of a jump across a branch cut, are

$$(1-x)^{\alpha}(1+x)^{\beta} P_k^{(\alpha,\beta)}(x) = \frac{1}{\pi i}\lim_{\epsilon\to 0}\left[(x-i\epsilon-1)^{\alpha}(x-i\epsilon+1)^{\beta} Q_k^{(\alpha,\beta)}(x-i\epsilon) - (x+i\epsilon-1)^{\alpha}(x+i\epsilon+1)^{\beta} Q_k^{(\alpha,\beta)}(x+i\epsilon)\right], \tag{7.9}$$

$$x^{\alpha}\exp(-x)\, L_k^{(\alpha)}(x) = \frac{\Gamma(k+\alpha+1)}{2\pi i}\left[\left(xe^{-i\pi}\right)^{\alpha} U\left(k+\alpha+1, \alpha+1, xe^{-i\pi}\right) - \left(xe^{i\pi}\right)^{\alpha} U\left(k+\alpha+1,\alpha+1,xe^{i\pi}\right)\right]. \tag{7.10}$$

Formula (7.9) is valid for x real in $-1 < x < 1$. The function $Q_k^{(\alpha,\beta)}(z)$ that appears in (7.9) is the second (irregular) solution of the differential equation for Jacobi polynomials. The function $(z-1)^\alpha (z+1)^\beta Q_k^{(\alpha,\beta)}(z)$ is analytic in the complex z plane cut along $[-1,+1]$. It can be conveniently defined by its relation to the hypergeometric function:

$$(z-1)^\alpha (z+1)^\beta Q_k^{(\alpha,\beta)}(z) = \frac{\Gamma(\alpha+k+1)\Gamma(\beta+k+1)2^{\alpha+\beta+k}}{\Gamma(\alpha+\beta+2k+2)(z-1)^{k+1}} \times {}_2F_1\left(k+1,\alpha+k+1;\alpha+\beta+2k+2;\frac{2}{1-z}\right). \quad (7.11)$$

Formula (7.10) is valid for x real and positive. The function $U(a,c,z)$ that appears in (7.9) is the second (irregular) solution of the differential equation for Laguerre polynomials. It is analytic in the complex z plane cut along $[-\infty,0]$; it has a branch point at 0 and a combination of a branch point and an essential singularity at ∞. It can be conveniently defined by the integral representation

$$U(a,c,z) = \frac{1}{\Gamma(a)}\int_0^\infty \exp(-zt)\, t^{a-1}(1+t)^{c-a-1}\, dt. \quad (7.12)$$

The contour integrals for $I_k^{(J;\alpha,\beta)}$ and $I_k^{(L;\alpha)}$ that can be obtained from these are

$$I_k^{(J;\alpha,\beta)} = \frac{1}{\pi i}\int_{C_J}\left[(1-z)^{-\alpha/2}(1+z)^{-\beta/2} f^{(J)}(z)\right] \times Q_k^{(\alpha,\beta)}(z)(z-1)^\alpha (z+1)^\beta\, dz, \quad (7.13)$$

$$I_k^{(L;\alpha)} = \frac{\Gamma(k+\alpha+1)}{2\pi i}\int_{C_L}\left[z^{-\alpha/2} f^{(L)}(z)\right]\left(ze^{-i\pi}\right)^\alpha \times U\left(k+\alpha+1,\alpha+1,ze^{-i\pi}\right)\exp(z/2)\, dz + \int_{x_0}^\infty f^{(L)}(x) L_k^{(\alpha)}(x)\, x^{\alpha/2}\exp(-x/2)\, dx. \quad (7.14)$$

The contours C_J and C_L are sketched in Figs. 5 and 6. The derivation of (7.13) and (7.14) from (7.6) and (7.8)–(7.10) assumes that $(1-z)^{-\alpha/2}(1+z)^{-\beta/2} f^{(J)}(z)$ is an analytic function of z within and on C_J and that $z^{-\alpha/2} f^{(L)}(z)$ is an analytic function of z within and on C_L.

The convergence of expansions of analytic functions in Jacobi, Laguerre, and Hermite series is discussed in Chap. IX of the work of Szegö [27]. The convergence of the Jacobi series (7.1) is similar to the convergence of Taylor and Laurent series, except that ellipses take the place of circles. Szegö shows that for $(1-z)^{-\alpha/2}(1+z)^{-\beta/2} f^{(J)}(z)$ analytic within the ellipse $\mathrm{Re}(z) = \frac{1}{2}\left(R+R^{-1}\right)\cos(\theta)$, $\mathrm{Im}(z) = \frac{1}{2}\left(R-R^{-1}\right)\sin(\theta)$, $0 \le \theta < 2\pi$, $R>1$, the series (7.1) converges to $f^{(J)}(z)$ for z inside the ellipse. If R has the largest value for which $(1-z)^{-\alpha/2}(1+z)^{-\beta/2} f^{(J)}(z)$ is analytic inside the ellipse, then the dominant part of the large k behavior of the expansion coefficients $c_k^{(J;\alpha,\beta)}$ in (7.1) is R^{-k}. This is the analog of the well known fact that Taylor series coefficients decrease like R^{-k} where R is the radius of convergence. For example, if the singularity that limits the size of the ellipse lies at $z=2$, the coefficients $c_k^{(J;\alpha,\beta)}$ decrease like R^{-k} with $R = |z+\sqrt{z^2-1}| = 2+\sqrt{3} \approx 3.732$. A more detailed description of the asymptotic behavior of the $c_k^{(J;\alpha,\beta)}$ can be obtained by the methods used above for Hermite series and below for a Laguerre series example. The situation for Laguerre and Hermite series is similar, except that the ellipse is replaced by a parabola with its focus at the origin for Laguerre series and by a strip symmetrically placed about the real axis for Hermite series.

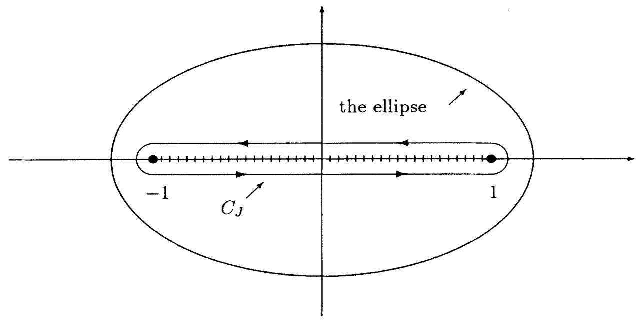

FIG. 5. Integration contour C_J and the ellipse of analyticity $\mathrm{Re}(z) = \frac{1}{2}\left(R+R^{-1}\right)\cos(\theta)$, $\mathrm{Im}(z) = \frac{1}{2}\left(R-R^{-1}\right)\sin(\theta)$, $0 \le \theta < 2\pi$, $R>1$ for Jacobi polynomial expansions.

As an example, consider the expansion of the function

$$f^{(L)}(x) = (x+c)^\nu \exp(-\gamma x) \quad (7.15)$$

in a Laguerre series of the form (7.2) with $\alpha = 0$. This example has been chosen because it has a branch point at $-c$, together with the exponential falloff that is typical of

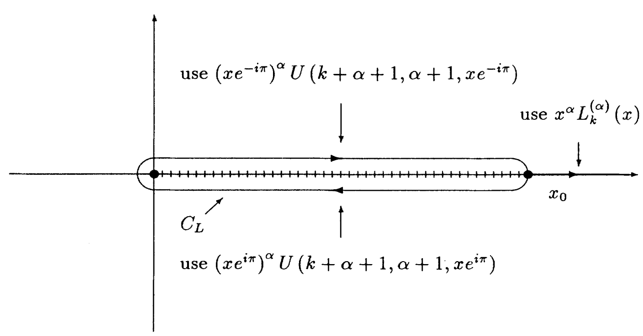

FIG. 6. Integration contour C_L for generalized Laguerre polynomial expansions.

bound state wave functions when the interaction vanishes at infinity. When $\gamma < \frac{1}{2}$, the integrand of the contour integral over C_L decays exponentially as $z \to -\infty$, the point x_0 can be chosen to lie at the saddle point $z_s = 4\left(k+\frac{1}{2}\right)\zeta_s$ where ζ_s is given by (7.19) below, and the contour C_L can be replaced by the contours shown in Fig. 7. When $\gamma > \frac{1}{2}$, the integrand of the contour integral over C_L decays exponentially as $z \to \infty$, the point x_0 can be chosen to lie at $+\infty$, and the contour C_L can be replaced by the contours shown in Fig. 8.

For k large, the asymptotic approximation

$$\begin{aligned} U\left[k+1,1,-4\left(k+\tfrac{1}{2}\right)\zeta\right] &\sim 2^{-1/2}\pi^{1/2}(k!)^{-1}\left(k+\tfrac{1}{2}\right)^{-1/2}(-\zeta)^{-1/4}(1-\zeta)^{-1/4} \\ &\quad\times\exp\Bigg(-2\left(k+\tfrac{1}{2}\right)\left\{\zeta+(-\zeta)^{1/2}(1-\zeta)^{1/2}\right. \\ &\qquad\left.+\ln\left[(-\zeta)^{1/2}+(1-\zeta)^{1/2}\right]\right\}\Bigg) \end{aligned} \tag{7.16}$$

can be used for U. The approximation (7.16), which is valid for k large and ζ not too close to the origin or to the turning point at $\zeta = 1$, can be obtained by constructing the Liouville-Green approximation to the solution of Whittaker's equation and using the connection between the function U and the Whittaker functions. Asymptotic expansions of confluent hypergeometric and Whittaker functions are discussed by Erdélyi and Swanson [28], Skovgarrd [29], and Olver (see [24], pp. 412–413, Examples 7.3 and 7.4; pp. 446–447, Example 4.6). The approximation (7.16), and a change of variables from z to $\zeta = \frac{1}{4}\left(k+\frac{1}{2}\right)^{-1} z$, brings the integral over C_L in (7.14) to the saddle point form $\int g(\zeta)\exp\left[-2\left(k+\frac{1}{2}\right)h(\zeta)\right]d\zeta$ with

$$\begin{aligned} g(\zeta) &= -2^{2\nu+1}(2\pi)^{-1/2}\, i\left(k+\tfrac{1}{2}\right)^{(2\nu+1)/2} \\ &\quad\times(-\zeta)^{-1/4}(1-\zeta)^{-1/4}\left[\zeta+\tfrac{1}{4}\left(k+\tfrac{1}{2}\right)^{-1}c\right]^{\nu}, \end{aligned} \tag{7.17}$$

$$\begin{aligned} h(\zeta) &= 2\gamma\zeta+(-\zeta)^{1/2}(1-\zeta)^{1/2} \\ &\quad+\ln\left[(-\zeta)^{1/2}+(1-\zeta)^{1/2}\right]. \end{aligned} \tag{7.18}$$

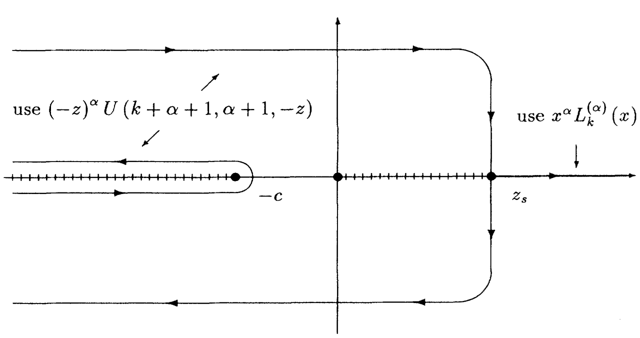

FIG. 7. Integration contours for the example when $\gamma < \frac{1}{2}$.

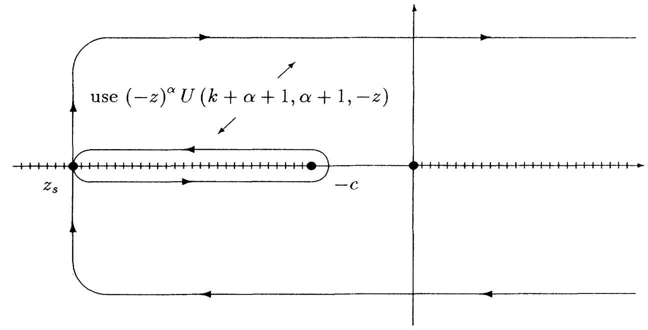

FIG. 8. Integration contours for the example when $\gamma > \frac{1}{2}$.

The integrand has a saddle point at the zero of $h'(\zeta)$, which lies at

$$\zeta_s = \left(1-4\gamma^2\right)^{-1}. \tag{7.19}$$

Application of the saddle point formula (6.8) with $w = -2\left(k+\frac{1}{2}\right)h$ yields a contribution $c_k^{(1)}$ to the expansion coefficient $c_k^{(L;0)} = I_k^{(L;0)}$, which is given by

$$\begin{aligned} c_k^{(1)} &= \left[\frac{2\Gamma(\nu+1)}{1+2\gamma}\right]\left[\frac{4}{1-4\gamma^2}\right]^{\nu}(-1)^k\binom{\nu+k}{k} \\ &\quad\times\left(\frac{1-2\gamma}{1+2\gamma}\right)^k\left[1+O\left(k^{-1}\right)\right],\quad \gamma<\tfrac{1}{2} \end{aligned} \tag{7.20}$$

$$\begin{aligned} c_k^{(1)} &= \left[\frac{2\Gamma(\nu+1)\cos(\pi\nu)}{1+2\gamma}\right]\left[\frac{4}{4\gamma^2-1}\right]^{\nu}\binom{\nu+k}{k} \\ &\quad\times\left(\frac{2\gamma-1}{2\gamma+1}\right)^k\left[1+O\left(k^{-1}\right)\right],\quad \gamma>\tfrac{1}{2}. \end{aligned} \tag{7.21}$$

There is an additional contribution to the asymptotics from the neighborhood of the branch point at $\zeta = -\frac{1}{4}\left(k+\frac{1}{2}\right)^{-1}c$. For k large, the integrand decreases so rapidly as ζ moves away from the branch point that only the neighborhood of the branch point matters. Small ζ approximations and the change of variables $(-\zeta)^{1/2} = \frac{1}{2}\left(k+\frac{1}{2}\right)^{-1/2}c^{1/2}+\frac{1}{4}\left(k+\frac{1}{2}\right)^{-1}s$ bring $\int g(\zeta)\exp\left[-2\left(k+\frac{1}{2}\right)w(\zeta)\right]d\zeta$ to the form

$$\begin{aligned} &\tfrac{1}{2}\pi^{-1/2} i c^{(2\nu+1)/4}\left(k+\tfrac{1}{2}\right)^{-(2\nu+3)/4} \\ &\quad\times\exp\left\{\gamma c-2\left[\left(k+\tfrac{1}{2}\right)c\right]^{1/2}\right\}\int(-s)^{\nu}\exp(-s)\,ds. \end{aligned} \tag{7.22}$$

The integral over s in (7.22) is a loop integral that can be recognized as Hankel's integral representation for $-2\pi i/\Gamma(-\nu)$. Inserting this in (7.22) yields, for the contribution from the branch point, the result

$$c_k^{(2)} = \frac{\pi^{1/2} c^{\nu+1}}{\Gamma(-\nu)} \left[c\left(k+\tfrac{1}{2}\right)\right]^{-(2\nu+3)/4} \times \exp\left\{\gamma c - 2\left[\left(k+\tfrac{1}{2}\right)c\right]^{1/2}\right\}\left[1+O\left(k^{-1/2}\right)\right]. \tag{7.23}$$

The procedure that led to (7.23) can be justified via an appeal to Barnes's lemma, which is better known as Watson's lemma for loop integrals (the theorem in asymptotic analysis that is known as Watson's lemma is usually attributed to Watson [30]. However, Wyman and Wong [31] have pointed out that Watson's lemma can be regarded as a special case of an earlier theorem of Barnes [32] (see also [22–24]).

The result (7.23) for the branch point contribution is correct only if $(k+1)c$ is large; thus the result for $c = 0$ cannot be obtained by taking the $c \to 0$ limit of (7.23). This restriction arises from a breakdown of the asymptotic formula (7.16) for U when $(k+1)\zeta$ is small. It can be cured by using a more complex asymptotic formula for U that remains valid as $\zeta \to 0$. This formula, which can be obtained from results given by Olver (see [24], pp. 446–447, Example 4.6), is

$$U\left[k+1, 1, -4\left(k+\tfrac{1}{2}\right)\zeta\right] \sim 2\,(k!)^{-1}(-\zeta)^{-1/4}(1-\zeta)^{-1/4} \times \exp\left[-2\left(k+\tfrac{1}{2}\right)\zeta\right]\xi^{1/4} K_0\left[4\left(k+\tfrac{1}{2}\right)^{1/2}\xi^{1/2}\right], \tag{7.24}$$

$$\xi^{1/2} = \tfrac{1}{2}\left\{(-\zeta)^{1/2}(1-\zeta)^{1/2} + \ln\left[(-\zeta)^{1/2} + (1-\zeta)^{1/2}\right]\right\}. \tag{7.25}$$

The function K_0 that appears in (7.24) is a modified Bessel function of the third kind in standard notation (see [11], p. 5; [12], pp. 66–67; or [16], pp. 374–375). The form that replaces (7.22) when (7.24) is used is

$$\pi^{-1} i \left(\frac{c}{k+\frac{1}{2}}\right)^{(\nu+1)/2} \exp(\gamma c) \times \int (-s)^{\nu} K_0\left[4\left(k+\tfrac{1}{2}\right)(-\zeta)^{1/2}\right] ds, \tag{7.26}$$

$$-\zeta = \tfrac{1}{4}\left[\left(k+\tfrac{1}{2}\right)^{-1} c + \left(k+\tfrac{1}{2}\right)^{-3/2} c^{1/2} s\right]. \tag{7.27}$$

The integration over s can be performed with the aid of the integral representation

$$K_\nu\left(2z^{1/2}\right) = \tfrac{1}{2} z^{-\nu/2} \int_0^\infty \exp\left(-zt - t^{-1}\right) t^{-\nu-1}\, dt \tag{7.28}$$

for the modified Bessel function of the third kind [see [11], p. 82, Eq. (23), or [12], p. 85]. Equation (7.28) is used for K_0, the orders of integration are interchanged, the integration over s is performed, and (7.28) is used again to recognize that the remaining integral over t is a $K_{\nu+1}$. The result is

$$c_k^{(2)} = \frac{2}{\Gamma(-\nu)}\left(\frac{c}{k+\frac{1}{2}}\right)^{(\nu+1)/2} \times K_{\nu+1}\left[2\sqrt{\left(k+\tfrac{1}{2}\right)c}\right]\left[1+O\left(k^{-1/2}\right)\right]. \tag{7.29}$$

The large z approximation $K_{\nu+1}(z) \approx \pi^{1/2}(2z)^{-1/2}\exp(-z)$ can be used to show that (7.29) reduces to (7.23) when $(k+\frac{1}{2})c$ is large. The asymptotic behavior of the expansion coefficient $c_k^{(L;0)} = I_k^{(L;0)}$ is given by the sum of the saddle point and branch point contributions:

$$c_k^{(L;0)} = I_k^{(L;0)} = c_k^{(1)} + c_k^{(2)}. \tag{7.30}$$

If $k \to \infty$ with γ held fixed, the contribution $c_k^{(1)}$ becomes negligible compared to $c_k^{(2)}$ for sufficiently large k. However, for any fixed large k, there is always a value of γ for which $c_k^{(1)}$ and $c_k^{(2)}$ have comparable magnitude. Thus both terms must be kept if the approximation is to be uniformly valid in γ. For $\gamma < \frac{1}{2}$, keeping the two terms comparable as k gets large requires letting γ get small. For $\gamma > \frac{1}{2}$, keeping the two terms comparable as k gets large requires letting γ get large. There is a difficulty in this case: when γ gets large, the saddle point [at $(1-4\gamma^2)^{-1}$] gets close to the branch point [at $-\frac{1}{4}(k+\frac{1}{2})^{-1}c$], the asymptotic analysis breaks down, and the more complicated approximation appropriate to a saddle point near an amplitude critical point (see [22], pp. 380–387) must be used. Since this section is intended to be illustrative rather than exhaustive, the resolution of this difficulty will be left as an exercise for the reader.

The asymptotic behavior of expansion coefficients can also be derived from a generating function. Although all of the classical orthogonal polynomials have generating functions, the method will be developed in detail only for the Laguerre polynomials, which have the generating function

$$(1-w)^{-\alpha-1}\exp\left(-\frac{wz}{1-w}\right) = \sum_{k=0}^{\infty} L_k^{(\alpha)}(z)\, w^k. \tag{7.31}$$

Introduce a generating function $g^{(L;\alpha)}(w)$ for the expansion coefficients $c_k^{(L;\alpha)}$ via

$$g^{(L;\alpha)}(w) = \sum_{k=0}^{\infty} c_k^{(L;\alpha)} w^k. \tag{7.32}$$

Equation (7.31) can be used to show that

$$g^{(L;\alpha)}(w) = (1-w)^{-\alpha-1} G^{(L;\alpha)}\left[\frac{(1+w)}{2(1-w)}\right], \tag{7.33}$$

where $G^{(L;\alpha)}$ is the Laplace transform

$$G^{(L;\alpha)}(\lambda) = \int_0^\infty x^{\alpha/2} f^{(L)}(x)\exp(-\lambda x)\, dx. \tag{7.34}$$

The asymptotic analysis of the expansion coefficient $c_k^{(L;\alpha)}$ begins with the Cauchy integral for $c_k^{(L;\alpha)}$, which is

$$c_k^{(L;\alpha)} = \frac{1}{2\pi i} \int_C w^{-k-1} g^{(L;\alpha)}(w)\, dw. \tag{7.35}$$

The contour C, which is a small circle that runs counterclockwise around the origin, is deformed to give integrals that can be evaluated via standard methods for the asymptotic evaluation of integrals. The function $f^{(L)}$ of Eq. (7.15) will again be used as an example. In this case,

$$g^{(L;0)}(w) = c^{\nu+1}(1-w)^{-1} U[1, \nu+2, t(w)], \tag{7.36}$$

$$t(w) = \frac{(1+2\gamma)c + (1-2\gamma)cw}{2(1-w)}. \tag{7.37}$$

The special case of U that appears in (7.36) has the properties

$$U(1, \nu+2, t) = \Gamma(\nu+1) t^{-\nu-1} \exp(t) - (\nu+1)^{-1} \times {}_1F_1(1, \nu+2, t), \tag{7.38}$$

$$U(1, \nu+2, t) = \sum_{k=0}^{K} (-1)^k (-\nu)_k t^{-k-1} + O\left(t^{-K-2}\right)$$

$$\text{for } t \to \infty \text{ in } -\tfrac{3}{2}\pi < \arg t < \tfrac{3}{2}\pi. \tag{7.39}$$

The convergent representation (7.38) of this U shows that it is analytic except for a branch point at $t = 0$ and a combination of a branch point and an essential singularity at $t = \infty$. It follows that the generating function $g^{(L;0)}(w)$ has a branch point on the negative real axis at $w = (2\gamma-1)^{-1}(2\gamma+1)$, which is on the negative real axis for $\gamma < \frac{1}{2}$ and on the positive real axis for $\gamma > \frac{1}{2}$. It has a combination of a branch point and an essential singularity on the positive real axis at $w = 1$. The associated branch cuts are shown in Figs. 9 and 10. Consider first the case $\gamma < \frac{1}{2}$ depicted in Fig. 9. The contour C is deformed into the sum of the two contours C_1 and C_2

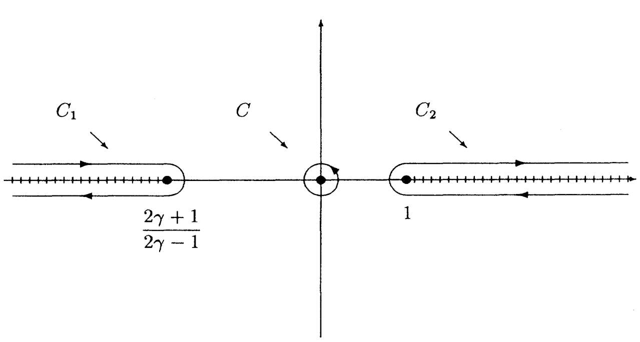

FIG. 9. The generating function method for the example when $\gamma < \frac{1}{2}$.

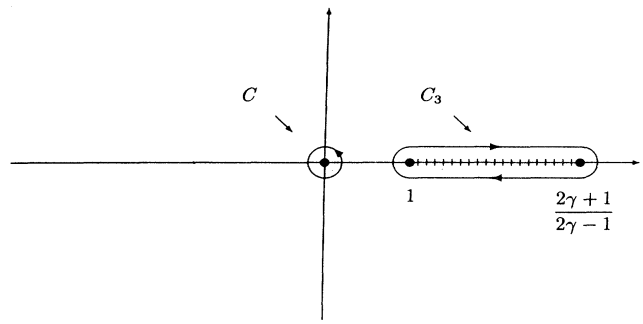

FIG. 10. The generating function method for the example when $\gamma > \frac{1}{2}$.

that run clockwise around the branch cuts. The expansion coefficient is then given by (7.30) with

$$c_k^{(j)} = \frac{1}{2\pi i} \int_{C_j} w^{-k-1} g^{(L;\alpha)}(w)\, dw, \quad j = 1, 2. \tag{7.40}$$

The asymptotic behavior of $c_k^{(1)}$ can be extracted in straightforward fashion via the method of Darboux (see [24], pp. 309–315,321, or [23], pp. 116–122). The result is again (7.20). The contribution $c_k^{(2)}$ requires a somewhat different strategy. The first step writes it as an integral along the real axis from $+1$ to $+\infty$ of the jump across the branch cut, which comes from the term $\Gamma(\nu+1) t^{-\nu-1} \exp(t)$ in the representation (7.38) of U. Evaluating the jump yields

$$c_k^{(2)} = \frac{1}{\Gamma(-\nu)} \int_0^\infty dx\, x^\nu \left[1 + \left(\tfrac{1}{2} - \gamma\right) x\right]^{-\nu-1} \times \exp\left[-\left(\tfrac{1}{2} - \gamma\right) c - (k+1)\ln(1+x) - cx^{-1}\right]. \tag{7.41}$$

The integrand in (7.41) has a saddle point at $x = [c/(k+1)]^{1/2}$. The asymptotics can be extracted via the saddle point method. The result is (7.23) with $k + \frac{1}{2}$ replaced by $k+1$; the difference due to this replacement is of the same order as the terms that have been neglected. The requirement that $(k+1)c$ be large must again be imposed. This requirement arises here because the saddle point approximation to (7.41) breaks down when the saddle point gets too close to the branch point at $x = 0$, which arises from the factor x^ν in the integrand. This breakdown can be cured relatively easily in this case by using small x approximations in the integrand of (7.41) to obtain

$$c_k^{(2)} \approx \frac{1}{\Gamma(-\nu)} \int_0^\infty dx\, x^\nu \exp\left[\gamma c - (k+1)x - cx^{-1}\right]. \tag{7.42}$$

The integral in (7.42) can be evaluated exactly by using (7.28) with $t = c^{-1}x$ and the fact that $K_{-\nu-1} = K_{\nu+1}$; the result is the approximation

$$c_k^{(2)} = \frac{2}{\Gamma(-\nu)} \left(\frac{c}{k+1}\right)^{(\nu+1)/2} \times K_{\nu+1}\left[2\sqrt{(k+1)\,c}\right]\left[1+O\left(k^{-1/2}\right)\right]. \quad (7.43)$$

Equation (7.43) is consistent with (7.29); the difference between the two is of the same order as the $O\left(k^{-1/2}\right)$ error term.

The analysis for the case $\gamma > \frac{1}{2}$ can be carried out by replacing the contour around the origin by the contour C_3 shown in Fig. 10. If the singularities at 1 and at $(2\gamma-1)^{-1}(2\gamma+1)$ are well separated, the evaluation of the contribution $c_n^{(2)}$ from the saddle point goes through as before and the contribution $c_k^{(1)}$ from the singularity at $(2\gamma-1)^{-1}(2\gamma+1)$ is negligible. However, as the two singularities approach each other, it becomes necessary to cope with an amplitude critical point near a saddle point, which is the difficulty that arose in the previous method.

The application of the generating function method to the example (7.15) exploited the fact that the Laplace transform (7.34) could be evaluated explicitly in terms of known, well-studied functions. Such explicit evaluation is not necessary, however, since the Laplace transform (7.34) is an integral representation for $G^{(L;\alpha)}$; integral representations normally provide the easiest starting point for determining the location of the singularities of a function and calculating expansions about those singularities. For the example (7.15), the singularity at $w = (2\gamma-1)^{-1}(2\gamma+1)$, which corresponds to $\lambda = -\gamma$, arises because this is the point at which the integral (7.34) no longer converges at infinity. The expansion about the singularity at $w = 1$, which corresponds to $\lambda = \infty$, can be obtained by using Watson's lemma [22–24] to deduce the large λ expansion of (7.34).

The generating function method outlined above has a very nice feature: if the singularity in the complex w plane that dominates the asymptotics is known, the analysis can be inverted to obtain a "convergence acceleration function" that builds in this singularity and has no other singularities in the finite complex w plane. The difference between the original $f^{(L)}(x)$ and this convergence acceleration function will have an expansion of the form (7.2), which converges faster than the expansion of $f^{(L)}(x)$. Examples can be found in the work of Forrey and Hill [33].

The contributions $c_k^{(1)}$ and $c_k^{(2)}$ exhibit two typical features. The most rapidly varying part, which is the factor $[(1-2\gamma)/(1+2\gamma)]^k$ in $c_k^{(1)}$ and the factor $\exp\{-2[c(k+\frac{1}{2})]^{1/2}\}$ in $c_k^{(2)}$, is determined by the location of the associated singularity. The next most important part, which is k^ν for $c_k^{(1)}$ and $(k+\frac{1}{2})^{-(2\nu+3)/4}$ for $c_k^{(2)}$, is determined by the nature of the singularity (i.e., by the value of ν). Additional terms in the expansions of the contributions $c_k^{(1)}$ and $c_k^{(2)}$ can be obtained by either of the two methods.

The results obtained for the example (7.15) can be extended in several ways. An expansion for the case in which the basis depends on a scale factor β can be obtained by replacing x by βx, c by βc, and γ by γ/β. Asymptotic formulas for a case in which the function being expanded has several well-separated branch point singularities can be obtained by adding up contributions of the form $c_k^{(2)}$ for each branch point; this is an example of the general principle that contributions to the asymptotics from well-separated singularities can be computed separately and added. A result for a logarithmic branch point can be obtained by taking a derivative with respect to the parameter ν.

ACKNOWLEDGMENTS

The introduction to asymptotic analysis given to the author by Professor Fritz Oberhettinger many years ago provided a set of tools and insights without which the present work could never have been performed. The author is indebted to John D. Morgan III for the suggestion that there should be contributions from the neighborhoods of the turning points of the basis functions for the Hamiltonian (1.8). This observation provided an essential starting point. The work was supported by National Science Foundation Grant Nos. PHY–8707970, PHY–9106797, and PHY–9406318.

APPENDIX A: DETAILS FOR THE $\cosh^{-2}$ POTENTIAL

This appendix outlines the derivation of the error formula (4.12)–(4.15) for the $\cosh^{-2}$ potential from (2.32). Two different derivations are given. The first uses best approximation in H^1, the second best approximation in L^2. Details that are common to both methods are presented first.

The computations begin with the kinetic and potential energy matrix elements, which are defined by

$$T_{k,\ell} = \tfrac{1}{2}\int_{-\infty}^{\infty}\left[\frac{d}{dz}e_{2k}(\alpha;z)\right]\left[\frac{d}{dz}e_{2\ell}(\alpha;z)\right]dz, \quad (A1)$$

$$V_{k,\ell} = -\int_{-\infty}^{\infty} e_{2k}(\alpha;z)\,\frac{1}{\cosh^2(z)}\,e_{2\ell}(\alpha;z)\,dz. \quad (A2)$$

The kinetic energy matrix elements $T_{k,\ell}$ are given explicitly by

$$T_{k,\ell} = \tfrac{1}{4}\alpha^2\Big\{-\left[(2\ell+2)(2\ell+1)\right]^{1/2}\delta_{k,\ell+1} + (4\ell+1)\,\delta_{k,\ell} - \left[2\ell\,(2\ell-1)\right]^{1/2}\delta_{k,\ell-1}\Big\}. \quad (A3)$$

There does not appear to be any simple formula for the potential energy matrix elements $V_{k,\ell}$; the values of the $V_{k,\ell}$ that are used in the variational calculation are obtained via Stenger's numerical integration method

[34–36]. However, the $V_{k,\ell}$ do have the following simple asymptotic formula:

$$V_{k,\ell} = -\frac{2\alpha}{\pi}(-1)^{k+\ell}\left[(4k+1)(4\ell+1)\right]^{-1/4} \times\left[\frac{\theta_{k,\ell}}{\sinh(\theta_{k,\ell})}\right] \times\left\{1+\frac{(\pi\alpha)^2 f(\theta_{k,\ell})}{\left[(4k+1)(4\ell+1)\right]^{1/2}} +O\left[\frac{1}{\min(k,\ell)}\right]\right\}, \tag{A4}$$

where

$$\theta_{k,\ell} = \tfrac{1}{2}\pi\left[(4k+1)^{1/2}-(4\ell+1)^{1/2}\right], \tag{A5}$$

$$f(\theta) = \tfrac{1}{48}\sinh^{-3}(\theta)\left\{\theta\cosh(\theta)\left[6+\sinh^2(\theta)\right] -3\sinh(\theta)\left[2+\sinh^2(\theta)\right]\right\}. \tag{A6}$$

The asymptotic formula (A4) can be derived as follows. Because $V_{k,\ell}$ is symmetric under interchange of k and ℓ, it is sufficient to consider the case $k \le \ell$. The derivation begins by using (2.3) for the factor $e_{2\ell}(\alpha;z)$ in the integrand. The factor $e_{2k}(\alpha;z)$ is left as is. The contour is deformed into the upper half plane for the term that contains $e_{2\ell}^{(+)}(\alpha;z)$ and into the lower half plane for the term that contains $e_{2\ell}^{(-)}(\alpha;z)$. The potential $\cosh^{-2}(z)$ has second-order poles on the imaginary axis at $z=\frac{1}{2}\pi(2m+1)\pi i$, where m is an integer; calculating the contributions from these poles yields

$$V_{k,\ell} = 2\sum_{m=0}^{\infty}\frac{d}{dm}\left\{e_{2k}\left[\alpha;\tfrac{1}{2}(2m+1)\pi i\right]e_{2\ell}^{(+)}\left[\alpha;\tfrac{1}{2}(2m+1)\pi i\right]+e_{2k}\left[\alpha;-\tfrac{1}{2}(2m+1)\pi i\right]e_{2\ell}^{(-)}\left[\alpha;-\tfrac{1}{2}(2m+1)\pi i\right]\right\}. \tag{A7}$$

If $\theta_{k,\ell}$ is not too small, the sum over m in (A7) can be evaluated by using the relation (3.3) and the asymptotic formula (3.8) to approximate the integrand; this works because the summand in (A7) is very small by the time the asymptotic formula (3.8) breaks down. The sum over m can then be evaluated with the aid of the summation formula

$$\sum_{m=0}^{\infty}\left(m+\tfrac{1}{2}\right)^q\exp\left[-c\left(m+\tfrac{1}{2}\right)\right] = \left(-\frac{\partial}{\partial c}\right)^q\sum_{m=0}^{\infty}\exp\left[-c\left(m+\tfrac{1}{2}\right)\right] = \left(-\frac{\partial}{\partial c}\right)^q\frac{1}{2\sinh(c/2)}. \tag{A8}$$

If $\theta_{k,n}$ is small, the sum over m in (A7) varies slowly and can be evaluated with the aid of the Euler-Maclaurin sum formula, which is

$$\sum_{m=M}^{N}f(m) = \int_M^N f(x)\,dx+\tfrac{1}{2}f(M)+\tfrac{1}{2}f(N)+\sum_{n\ge1}\frac{1}{(2n)!}B_{2n}\left[f^{(2n-1)}(N)-f^{(2n-1)}(M)\right]. \tag{A9}$$

The B_{2n} in (A9) are Bernoulli numbers; the first few are $B_2=\frac{1}{6}$, $B_4=-\frac{1}{30}$, $B_6=\frac{1}{42}$, $B_8=-\frac{1}{30}$, $B_{10}=\frac{5}{66}$, $B_{12}=-\frac{691}{2730}$, and $B_{14}=\frac{7}{6}$. The Euler-Maclaurin sum formula requires only a knowledge of the summand in (A7) for $k=0$, which can be obtained from (3.8). A resummation with the aid of the generating function formula for the Bernoulli numbers, which is

$$\frac{z}{\exp(z)-1} = \sum_{n=0}^{\infty}B_n\frac{z^n}{n!}, \tag{A10}$$

again yields (A4).

The Euler-Maclaurin sum formula can be used to deduce summation formulas such as

$$\sum_{k=K+1}^{\infty}(4k+1)^{\ell/2}\exp\left[-c(4k+1)^{1/2}\right] = \exp\left[-c(4K+5)^{1/2}\right]\left\{\frac{1}{2c}(4K+5)^{(\ell+1)/2}+\left[\frac{1}{2}+\frac{(\ell+1)}{2c^2}\right](4K+5)^{\ell/2} +\left[\frac{c}{6}+\frac{\ell(\ell+1)}{2c^3}\right](4K+5)^{(\ell-1)/2}-\left[\frac{\ell}{6}-\frac{(\ell-1)\ell(\ell+1)}{2c^4}\right](4K+5)^{(\ell-2)/2}+O\left[K^{(\ell-3)/2}\right]\right\}. \tag{A11}$$

Summation formulas for sums with alternating signs can be obtained via summation by parts. Define the finite difference operator Δ_j in the usual way by

$$\Delta_j f(j) = f(j+1) - f(j) , \quad \text{(A12)}$$

where $f(j)$ is an arbitrary function of the integer variable j. The summation by parts formula, which is a finite-difference analog of the well-known integration by parts formula, is

$$\sum_{j=m}^{n} h(j)\,\Delta_j g(j) = g(n+1)\,h(n+1) - g(m)\,h(m) - \sum_{j=m}^{n} g(j+1)\,\Delta_j h(j) , \quad \text{(A13)}$$

where $g(j)$ and $h(j)$ are arbitrary functions of the integer variable j. The choice $g(j) = -\frac{1}{2}(-1)^j$ implies that $\Delta_j g(j) = (-1)^j$ and yields the formula

$$\sum_{j=m}^{n} (-1)^j h(j) = \tfrac{1}{2}(-1)^n h(n+1) + \tfrac{1}{2}(-1)^m h(m) - \tfrac{1}{2}\sum_{j=m}^{n} (-1)^j \Delta_j h(j) . \quad \text{(A14)}$$

Repeated summation by parts with the aid of (A14), followed by an evaluation of the finite differences via Taylor series expansions, yields summation formulas such as

$$\sum_{k=K+1}^{\infty} (-1)^k (4k+1)^{\ell/2} \exp\left[-c(4k+1)^{1/2}\right] = \tfrac{1}{2}(4K+5)^{\ell/2}(-1)^{K+1}\exp\left[-c(4K+5)^{1/2}\right] \times[1 + c(4K+5)^{-1/2} - \ell(4K+5)^{-1} + O(K^{-3/2})]. \quad \text{(A15)}$$

The constant c that appears in (A11) and (A15) must be positive. The summation formula (A15) can also be obtained by applying the Euler-Maclaurin sum formula to the odd k and even k terms separately.

The evaluation of the error when the best approximation in H^1 is used for $|\tilde{\psi}^{(B;K)}\rangle$ in (2.32) begins with the construction of asymptotic formulas for the elements $U_{k,\ell}$ of the upper triangular matrix that appears in (2.19). Because the kinetic energy matrix (A3) is tridiagonal, only $U_{k,k}$ and $U_{k,k+1}$ are nonzero and the Cholesky decomposition formulas (2.14) and (2.15) simplify to

$$U_{k,k+1} = T_{k,k+1}/U_{k,k}, \quad \text{(A16)}$$

$$U_{k,k} = \left[\left(T_{k,k} + \beta^2\right) - \left(T_{k-1,k}/U_{k-1,k-1}\right)^2\right]^{1/2} . \quad \text{(A17)}$$

A large k asymptotic expansion of $U_{k,k}$ can be obtained by looking for a series solution to (A17) of the form

$$U_{k,k} \sim (4k+1)^{1/2} \sum_{\ell=0}^{\infty} u_k (4k+1)^{-\ell} . \quad \text{(A18)}$$

Ambiguities that arise from multiple roots when solving for the coefficients u_k can be resolved and the correct root selected by comparison of the asymptotic results with numerical Cholesky decomposition. In the present case this happens only for u_1; it is necessary to choose between $+\frac{1}{2}\beta$ and $-\frac{1}{2}\beta$. The asymptotic expansion of $U_{k,k+1}$ can be obtained by inserting the asymptotic expansion of $U_{k,k}$ in (A16). The results are

$$U_{k,k} = \tfrac{1}{4}\sqrt{2}\alpha(4k+1)^{1/2} + \tfrac{1}{2}|\beta| + \tfrac{1}{8}\sqrt{2}\alpha^{-1}\left(\alpha^2 + 2\beta^2\right)(4k+1)^{-1/2} - \tfrac{1}{4}|\beta|(4k+1)^{-1} - \tfrac{1}{32}\sqrt{2}\alpha^{-3}\left(\alpha^2+2\beta^2\right)^2 \times (4k+1)^{-3/2} + O\left(k^{-2}\right) , \quad \text{(A19)}$$

$$U_{k,k+1} = -\tfrac{1}{4}\sqrt{2}\alpha(4k+1)^{1/2} + \tfrac{1}{2}|\beta| - \tfrac{1}{8}\sqrt{2}\alpha^{-1}\left(3\alpha^2 + 2\beta^2\right)(4k+1)^{-1/2} + \tfrac{1}{4}|\beta|(4k+1)^{-1} + \tfrac{1}{32}\sqrt{2}\alpha^{-3}\left(3\alpha^2+2\beta^2\right)^2 \times (4k+1)^{-3/2} + O\left(k^{-2}\right) . \quad \text{(A20)}$$

Asymptotic formulas for the elements $\left(U^{-1}\right)_{k,\ell}$ of the upper triangular matrix inverse to $U_{k,\ell}$ are needed for the computation of asymptotic formulas for the potential energy matrix elements $\langle\eta_k|V|\eta_\ell\rangle$ and the Gram matrix elements $\langle\eta_k|\eta_\ell\rangle$. Mathematical induction on m can be used to show that

$$\left(U^{-1}\right)_{k-m,k} = \frac{(-1)^m}{U_{k,k}} \prod_{n=0}^{m-1} \frac{U_{k-m+n,k-m+n+1}}{U_{k-m+n,k-m+n}} . \quad \text{(A21)}$$

The expression (A21) is valid whenever the kinetic energy matrix is tridiagonal so that only $U_{k,k}$ and $U_{k,k+1}$ are nonzero. It can be evaluated asymptotically by writing

$$(-1)^m \prod_{n=0}^{m-1} \frac{U_{k-m+n,k-m+n+1}}{U_{k-m+n,k-m+n}} = \exp\left[\sum_{n=0}^{m-1} \ln\left(-\frac{U_{k-m+n,k-m+n+1}}{U_{k-m+n,k-m+n}}\right)\right] . \quad \text{(A22)}$$

An asymptotic expansion of the logarithm on the right-hand side of (A22) that is valid for $k-m+n$ large can be worked out by expanding the logarithm in inverse powers of $(4k-4m+4n+1)^{1/2}$ with the aid of (A19) and (A20). The sum from $n=0$ to $n=m-1$ can then be performed with the aid of the Euler-Maclaurin sum formula. In this way it can be shown that

$$\left(U^{-1}\right)_{k,\ell} = 2^{3/2}\alpha^{-1}\left[(4\ell+1)(4k+1)\right]^{-1/4}\exp\left\{\alpha^{-1}2^{1/2}|\beta|\left[(4k+1)^{1/2}-(4\ell+1)^{1/2}\right]\right\}$$
$$\times\left\{1+\tfrac{7}{6}\left(\alpha^{-1}2^{1/2}|\beta|\right)^3\left[(4k+1)^{-1/2}-(4\ell+1)^{-1/2}\right]-\alpha^{-1}2^{1/2}|\beta|(4\ell+1)^{-1/2}+O\left(k^{-1}\right)\right\}. \quad \text{(A23)}$$

The desired asymptotic formulas for matrix elements with respect to the $|\eta_k\rangle$ can be calculated from (2.2), (2.7), (A4), (A23), and analogs of the sum formulas (A11) and (A15). The results are

$$\langle\eta_k|\eta_\ell\rangle = \frac{\sqrt{2}}{\alpha|\beta|}\left[(4k+1)(4\ell+1)\right]^{-1/4}\exp\left[-\alpha^{-1}2^{1/2}|\beta|\left|(4k+1)^{1/2}-(4\ell+1)^{1/2}\right|\right]\left[1+O\left(k^{-1/2}\right)+O\left(\ell^{-1/2}\right)\right], \quad \text{(A24)}$$

$$\langle\eta_k|V|\eta_\ell\rangle = -\frac{4}{\pi\alpha}(-1)^{k+\ell}\left[(4k+1)(4\ell+1)\right]^{-3/4}\left[\frac{\theta_{k,\ell}}{\sinh\left(\theta_{k,\ell}\right)}\right]\left[1+O\left(k^{-1/2}\right)+O\left(\ell^{-1/2}\right)\right]. \quad \text{(A25)}$$

The singularity and turning point contributions to $\hat{c}_k$ can be calculated from $\hat{c}_k = U_{k,k}c_k + U_{k,k+1}c_{k+1}$. The results are

$$\hat{c}_k^{(\mathrm{sing})} = (2\pi)^{1/2}\alpha^{3/2}(4k+1)^{1/4}(-1)^k\exp\left[-\tfrac{1}{2}\pi\alpha(4k+1)^{1/2}\right]$$
$$\times\left\{1-\tfrac{1}{2}\pi\alpha\left[1+\tfrac{1}{24}(\pi\alpha)^2\right](4k+1)^{-1/2}+\left[\tfrac{1}{2}+\tfrac{3}{16}(\pi\alpha)^2+\tfrac{1}{96}(\pi\alpha)^4\right.\right.$$
$$\left.\left.+\tfrac{1}{4608}(\pi\alpha)^6+2^{-1/2}\pi|\beta|+\alpha^{-2}\beta^2\right](4k+1)^{-1}+O\left(k^{-3/2}\right)\right\}, \quad \text{(A26)}$$

$$\hat{c}_k^{(\mathrm{TP})} = 2\alpha^{-1/2}\left(1+2^{1/2}|\beta|\right)(4k+1)^{-1/4}\exp\left[-\alpha^{-1}(4k+1)^{1/2}\right]$$
$$\times\left\{1-\left(\alpha^{-1}+\tfrac{1}{6}\alpha^{-3}\right)(4k+1)^{-1/2}+\left[-\tfrac{1}{2}+\tfrac{1}{4}\left(1+2^{3/2}|\beta|\right)\alpha^{-2}\right.\right.$$
$$\left.\left.+\tfrac{1}{6}\alpha^{-4}+\tfrac{1}{72}\alpha^{-6}\right](4k+1)^{-1}+O\left(k^{-3/2}\right)\right\}. \quad \text{(A27)}$$

The various contributions to $\langle\delta\psi^{(H^1;K)}|H-EI|\delta\psi^{(H^1;K)}\rangle$, which is the first term in the numerator of the error formula (2.32), can now be calculated. The easiest are the contributions to $\langle\delta\psi^{(H^1;K)}|T+\beta^2 I|\delta\psi^{(H^1;K)}\rangle$, which are just $\sum_{k=K+1}^{\infty}|\hat{c}_k|^2$ as a consequence of (2.8) and (2.11). Performing the sum over k with the aid of (A11) and (A15) yields

$$\sum_{k=K+1}^{\infty}|\hat{c}_k^{(\mathrm{sing})}|^2 = \alpha^2(4K+5)\exp\left[-\pi\alpha(4K+5)^{1/2}\right]\left\{1+\left[2(\pi\alpha)^{-1}-\tfrac{1}{24}(\pi\alpha)^3\right](4K+5)^{-1/2}\right.$$
$$\left.+\left[2(\pi\alpha)^{-2}-\tfrac{1}{12}(\pi\alpha)^2+\tfrac{1}{1152}(\pi\alpha)^6+2^{1/2}\pi|\beta|+2\alpha^{-2}\beta^2\right](4K+5)^{-1}+O\left(K^{-3/2}\right)\right\}, \quad \text{(A28)}$$

$$\sum_{k=K+1}^{\infty}|\hat{c}_k^{(\mathrm{TP})}|^2 = \left(1+2^{1/2}|\beta|\right)^2\exp\left[-2\alpha^{-1}(4K+5)^{1/2}\right]$$
$$\times\left\{1-\tfrac{1}{3}\alpha^{-3}(4K+5)^{-1/2}+\left[\left(-1+2^{1/2}|\beta|\right)\alpha^{-2}+\tfrac{1}{18}\alpha^{-6}\right](4K+5)^{-1}+O\left(K^{-3/2}\right)\right\}, \quad \text{(A29)}$$

$$\sum_{k=K+1}^{\infty}\left[\bar{\hat{c}}_k^{(\mathrm{sing})}\hat{c}_k^{(\mathrm{TP})}+\bar{\hat{c}}_k^{(\mathrm{TP})}\hat{c}_k^{(\mathrm{sing})}\right] = 2^{3/2}\pi^{1/2}\alpha\left(1+2^{1/2}|\beta|\right)(-1)^{K+1}\exp\left[-\left(\tfrac{1}{2}\pi\alpha+\alpha^{-1}\right)(4K+5)^{1/2}\right]$$
$$\times\left\{1-\left[\tfrac{1}{6}\alpha^{-3}+\tfrac{1}{48}(\pi\alpha)^3\right](4K+5)^{-1/2}+O\left(K^{-1}\right)\right\}, \quad \text{(A30)}$$

The contributions to $\langle\delta\psi^{(H^1;K)}|\delta\psi^{(H^1;K)}\rangle$ are

$$\sum_{k=K+1}^{\infty}\sum_{\ell=K+1}^{\infty}\bar{\hat{c}}_k^{(\mathrm{sing})}\hat{c}_\ell^{(\mathrm{sing})}\langle\eta_k|\eta_\ell\rangle = \frac{\pi\alpha^2}{|\beta|\sqrt{2}}\exp\left[-\pi\alpha(4K+5)^{1/2}\right]\left[1+O\left(K^{-1/2}\right)\right], \quad \text{(A31)}$$

$$\sum_{k=K+1}^{\infty}\sum_{\ell=K+1}^{\infty}\bar{\hat{c}}_k^{(\mathrm{TP})}\hat{c}_\ell^{(\mathrm{TP})}\langle\eta_k|\eta_\ell\rangle = \frac{\sqrt{2}}{\beta^2}\left(1+2^{1/2}|\beta|\right)\exp\left[-2\alpha^{-1}(4K+5)^{1/2}\right]\left[1+O\left(K^{-1/2}\right)\right], \quad \text{(A32)}$$

$$\sum_{k=K+1}^{\infty}\sum_{\ell=K+1}^{\infty}\left[\bar{\hat{c}}_k^{(\text{sing})}\hat{c}_\ell^{(\text{TP})}+\bar{\hat{c}}_k^{(\text{TP})}\hat{c}_\ell^{(\text{sing})}\right]\langle\eta_k|\eta_\ell\rangle = \frac{2\alpha\sqrt{\pi}}{|\beta|}(-1)^{K+1}\exp\left[-\left(\tfrac{1}{2}\pi\alpha+\alpha^{-1}\right)(4K+5)^{1/2}\right]\left[1+O\left(K^{-1/2}\right)\right]. \tag{A33}$$

The contributions to $\langle\delta\psi^{(H^1;K)}|V|\delta\psi^{(H^1;K)}\rangle$ are

$$\sum_{k=K+1}^{\infty}\sum_{\ell=K+1}^{\infty}\bar{\hat{c}}_k^{(\text{sing})}\hat{c}_\ell^{(\text{sing})}\langle\eta_k|V|\eta_\ell\rangle = -\frac{4\alpha}{\pi^2}\zeta\left(2,\tfrac{1}{2}\alpha+\tfrac{1}{2}\right)\exp\left[-\pi\alpha(4K+5)^{1/2}\right]\left[1+O\left(K^{-1/2}\right)\right], \tag{A34}$$

$$\sum_{k=K+1}^{\infty}\sum_{\ell=K+1}^{\infty}\bar{\hat{c}}_k^{(\text{TP})}\hat{c}_\ell^{(\text{TP})}\langle\eta_k|V|\eta_\ell\rangle = -\frac{4}{\pi\alpha^2}\left(1+2^{1/2}|\beta|\right)^2(4K+5)^{-2}\exp\left[-2\alpha^{-1}(4K+5)^{1/2}\right]\left[1+O\left(K^{-1/2}\right)\right], \tag{A35}$$

$$\sum_{k=K+1}^{\infty}\sum_{\ell=K+1}^{\infty}\left[\bar{\hat{c}}_k^{(\text{sing})}\hat{c}_\ell^{(\text{TP})}+\bar{\hat{c}}_k^{(\text{TP})}\hat{c}_\ell^{(\text{sing})}\right]\langle\eta_k|V|\eta_\ell\rangle = -2^{5/2}\pi^{-3/2}\left(1+2^{1/2}|\beta|\right)\zeta\left(2,\tfrac{1}{2}\alpha+\tfrac{1}{2}\right)(-1)^{K+1}(4K+5)^{-1}$$
$$\times\exp\left[-\left(\tfrac{1}{2}\pi\alpha+\alpha^{-1}\right)(4K+5)^{1/2}\right]\left[1+O\left(K^{-1/2}\right)\right]. \tag{A36}$$

The function $\zeta\left(2,\frac{1}{2}\alpha+\frac{1}{2}\right)$ that appears in (A34) is the Hurwitz zeta function, also known as the generalized zeta function, in standard notation (see [12], pp. 22–25, or [19], pp. 24–27). The result (4.12)–(4.15) for the error $\tilde{E}^{(\text{RR};K)}-E$ can now be assembled by adding up the contributions to $\langle\delta\psi^{(H^1;K)}|(H-EI)|\delta\psi^{(H^1;K)}\rangle$ from (A28)–(A30) and (A34), which are used with $\beta=2^{-1/2}$. The approximation $\langle\tilde{\psi}^{(B;K)}|\tilde{\psi}^{(B;K)}\rangle\approx 1$ is used for the denominator in (2.32). The methods used below to derive the result (4.12)–(4.15) via best approximation in L^2 can be used to show that the second term in the numerator of (2.32) does not contribute to the order to which the calculation has been carried. Formulas (A31)–(A33), (A35), and (A36) have been evaluated to one term to show that they do not contribute.

The evaluation of the error $\tilde{E}^{(\text{RR};K)}-E$ when the best approximation in L^2 is used for $|\tilde{\psi}^{(B;K)}\rangle$ in the error formula (2.32) begins with the evaluation of the first term of the numerator, which is $\langle\delta\psi^{(L^2;K)}|(H-EI)|\delta\psi^{(L^2;K)}\rangle$. Evaluation of the needed sums with the aid of (A11) and (A15) yields, for the kinetic energy contributions,

$$\sum_{k=K+1}^{\infty}\sum_{\ell=K+1}^{\infty}\bar{c}_k^{(\text{sing})}T_{k,\ell}c_\ell^{(\text{sing})} = \alpha^2(4K+5)\exp\left[-\pi\alpha(4K+5)^{1/2}\right]$$
$$\times\left\{1+\left[2(\pi\alpha)^{-1}+\tfrac{1}{2}\pi\alpha-\tfrac{1}{24}(\pi\alpha)^3\right](4K+5)^{-1/2}\right.$$
$$\left.+\left[2(\pi\alpha)^{-2}-\tfrac{1}{12}(\pi\alpha)^2-\tfrac{1}{48}(\pi\alpha)^4+\tfrac{1}{1152}(\pi\alpha)^6\right](4K+5)^{-1}+O\left(K^{-3/2}\right)\right\}, \tag{A37}$$

$$\sum_{k=K+1}^{\infty}\sum_{\ell=K+1}^{\infty}\bar{c}_k^{(\text{TP})}T_{k,\ell}c_\ell^{(\text{TP})} = \alpha(4K+5)^{1/2}\exp\left[-2\alpha^{-1}(4K+5)^{1/2}\right]$$
$$\times\left[1+\left(\alpha^{-1}-\tfrac{1}{3}\alpha^{-3}\right)(4K+5)^{-1/2}-\left(1+\tfrac{1}{2}\alpha^{-2}+\tfrac{1}{3}\alpha^{-4}-\tfrac{1}{18}\alpha^{-6}\right)(4K+5)^{-1}\right.$$
$$\left.-\left(\tfrac{1}{2}\alpha^{-1}+\tfrac{2}{3}\alpha^{-3}-\tfrac{13}{60}\alpha^{-5}-\tfrac{1}{18}\alpha^{-7}+\tfrac{1}{162}\alpha^{-9}\right)(4K+5)^{-3/2}+O\left(K^{-2}\right)\right], \tag{A38}$$

$$\sum_{k=K+1}^{\infty}\sum_{\ell=K+1}^{\infty}\left[\bar{c}_k^{(\text{sing})}T_{k,\ell}c_\ell^{(\text{TP})}+\bar{c}_k^{(\text{TP})}T_{k,\ell}c_\ell^{(\text{sing})}\right]$$
$$=(2\pi)^{1/2}\alpha^2(-1)^{K+1}(4K+5)^{1/2}\exp\left[-\left(\tfrac{1}{2}\pi\alpha+\alpha^{-1}\right)(4K+5)^{1/2}\right]$$
$$\times\left\{1-\left[\tfrac{1}{6}\alpha^{-3}-2\alpha^{-1}+\tfrac{1}{48}(\pi\alpha)^3\right](4K+5)^{-1/2}+\left[\tfrac{1}{72}\alpha^{-6}-\tfrac{1}{3}\alpha^{-4}-\tfrac{1}{4}\alpha^{-2}+\tfrac{1}{288}\pi^3-1\right.\right.$$
$$\left.\left.-\left(\tfrac{1}{24}\pi+\tfrac{1}{16}\right)(\pi\alpha)^2+\tfrac{1}{4608}(\pi\alpha)^6\right](4K+5)^{-1}+O\left(K^{-3/2}\right)\right\}, \tag{A39}$$

for the potential energy contributions

$$\sum_{k=K+1}^{\infty}\sum_{\ell=K+1}^{\infty}\bar{c}_k^{(\text{sing})}V_{k,\ell}c_\ell^{(\text{sing})} = -\frac{4\alpha}{\pi^2}\zeta\left(2,\tfrac{1}{2}\alpha+\tfrac{1}{2}\right)\exp\left[-\pi\alpha\left(4K+5\right)^{1/2}\right]\left[1+O\left(K^{-1/2}\right)\right], \tag{A40}$$

$$\sum_{k=K+1}^{\infty}\sum_{\ell=K+1}^{\infty}\bar{c}_k^{(\text{TP})}V_{k,\ell}c_\ell^{(\text{TP})} = -\frac{4}{\pi}\left(4K+5\right)^{-1}\exp\left[-2\alpha^{-1}\left(4K+5\right)^{1/2}\right]\left[1+O\left(K^{-1/2}\right)\right], \tag{A41}$$

$$\sum_{k=K+1}^{\infty}\sum_{\ell=K+1}^{\infty}\left[\bar{c}_k^{(\text{sing})}V_{k,\ell}c_\ell^{(\text{TP})}+\bar{c}_k^{(\text{TP})}V_{k,\ell}c_\ell^{(\text{sing})}\right]$$

$$= -2^{5/2}\pi^{-3/2}\alpha\zeta\left(2,\tfrac{1}{2}\alpha+\tfrac{1}{2}\right)\left(-1\right)^{K+1}\left(4K+5\right)^{-1/2}\exp\left[-\left(\tfrac{1}{2}\pi\alpha+\alpha^{-1}\right)\left(4K+5\right)^{1/2}\right]\left[1+O\left(K^{-1/2}\right)\right], \tag{A42}$$

and for the normalization contributions

$$\sum_{k=K+1}^{\infty}|c_k^{(\text{sing})}|^2 = 2\exp\left[-\pi\alpha\left(4K+5\right)^{1/2}\right]\left[1+O\left(K^{-1/2}\right)\right], \tag{A43}$$

$$\sum_{k=K+1}^{\infty}|c_k^{(\text{TP})}|^2 = 2\exp\left[-2\alpha^{-1}\left(4K+5\right)^{1/2}\right]\left[1+\left(2\alpha^{-1}-\tfrac{1}{3}\alpha^{-3}\right)\left(4K+5\right)^{-1/2}\right.$$
$$\left.+\left(\alpha^{-2}-\tfrac{2}{3}\alpha^{-4}+\tfrac{1}{18}\alpha^{-6}\right)\left(4K+5\right)^{-1}+O\left(K^{-3/2}\right)\right], \tag{A44}$$

$$\sum_{k=K+1}^{\infty}\left[\bar{c}_k^{(\text{sing})}c_k^{(\text{TP})}+\bar{c}_k^{(\text{TP})}c_k^{(\text{sing})}\right]$$

$$= 2^{5/2}\pi^{1/2}\left(-1\right)^{K+1}\left(4K+5\right)^{-1/2}\exp\left[-\left(\tfrac{1}{2}\pi\alpha+\alpha^{-1}\right)\left(4K+5\right)^{1/2}\right]\left[1+O\left(K^{-1/2}\right)\right]. \tag{A45}$$

The first numerator term $\langle\delta\psi^{(L^2;K)}|\left(H-EI\right)|\delta\psi^{(L^2;K)}\rangle$ in (2.32) can now be assembled by adding up the contributions from (A37)–(A45). Formulas (A43)–(A45) can be used to show that the denominator $\langle\tilde{\psi}^{(L^2;K)}|\tilde{\psi}^{(L^2;K)}\rangle$ in (2.32) can be approximated by 1. A comparison of the dominant contributions to the first numerator term, which come from (A37)–(A39), with (4.12)–(4.15) shows that the contributions to the error $\tilde{E}^{(\text{RR};K)}-E$ do not all come from the first numerator term in (2.32) when best approximation in L^2 is used; the second numerator term in (2.32) must also be evaluated in this case.

The evaluation of the second numerator term in (2.32) requires an asymptotic evaluation of the inverse $A\left(\mu\right)$, which is introduced in (2.29). This evaluation begins with the asymptotic evaluation of the upper triangular matrix $W_{k,\ell}$ from the generalized Cholesky decomposition formulas (2.33)–(2.37). Because the kinetic energy matrix element $T_{k,\ell}$ dominates for k and ℓ large, this evaluation is similar to the evaluation of $U_{k,\ell}$ given above. The result is

$$W_{k,\ell}\approx U_{k,\ell}+\left(4k+1\right)^{-1/2}2^{-1/2}\alpha^{-1}V_{k,\ell}\ \text{ for }\ k\leq\ell. \tag{A46}$$

In applications of (A46), $U_{k,\ell}$ is replaced by the asymptotic expansion recorded in (A19) and (A20) and $V_{k,\ell}$ is replaced by the asymptotic expansion (A4). It can be shown with the aid of (A16), (A21), and (A46) that the second numerator term in (2.32) is given with sufficient accuracy by the approximation

$$-\langle\delta\psi^{(L^2;K)}|\left(H-EI\right)\tilde{P}_\perp A\left(\mu\right)\tilde{P}_\perp\left(H-EI\right)|\delta\psi^{(L^2;K)}\rangle$$
$$\approx -|U_{K,K+1}c_{K+1}|^2\left[1-\left(4K+5\right)^{-1/2}2^{1/2}\sum_{k=0}^{K}V_{K,k}\left(U^{-1}\right)_{k,K}\right]$$
$$-U_{K,K+1}\sum_{k=0}^{K}\sum_{\ell=K+1}^{\infty}\left(U^{-1}\right)_{k,K}V_{k,\ell}\left(\overline{c_{K+1}}c_\ell+\overline{c_\ell}c_{K+1}\right). \tag{A47}$$

The evaluation of the various contributions to (A47) is straightforward. The pieces that contribute to the order to which the calculations have been carried are

$$|U_{K,K+1}c_{K+1}^{(\mathrm{sing})}|^2 = \alpha^2 (4K+5) \exp\left[-\pi\alpha (4K+5)^{1/2}\right] \times \left\{\tfrac{1}{2}\pi\alpha (4K+5)^{-1/2} - \left[\pi + \tfrac{1}{48}(\pi\alpha)^4\right](4K+5)^{-1} + O\left(K^{-3/2}\right)\right\}, \quad (A48)$$

$$|U_{K,K+1}c_{K+1}^{(\mathrm{TP})}|^2 = \alpha (4K+5)^{1/2} \exp\left[-2\alpha^{-1}(4K+5)^{1/2}\right] \times \left\{1 - \left(2\alpha^{-1} + \tfrac{1}{3}\alpha^{-3}\right)(4K+5)^{-1/2} - \left(1 - \tfrac{3}{2}\alpha^{-2} - \tfrac{2}{3}\alpha^{-4} - \tfrac{1}{18}\alpha^{-6}\right) \times (4K+5)^{-1} - \left(\tfrac{1}{2}\alpha^{-1} - \tfrac{1}{3}\alpha^{-3} + \tfrac{9}{20}\alpha^{-5} + \tfrac{1}{9}\alpha^{-7} + \tfrac{1}{162}\alpha^{-9}\right)(4K+5)^{-3/2} + O\left(K^{-2}\right)\right\}, \quad (A49)$$

$$|U_{K,K+1}|^2 \left[\bar{c}_{K+1}^{(\mathrm{sing})} c_{K+1}^{(\mathrm{TP})} + \bar{c}_{K+1}^{(\mathrm{TP})} c_{K+1}^{(\mathrm{sing})}\right]$$

$$= (2\pi)^{1/2}\alpha^2(-1)^{K+1}(4K+5)^{1/2}\exp\left[-\left(\tfrac{1}{2}\pi\alpha + \alpha^{-1}\right)(4K+5)^{1/2}\right] \times \left\{1 - \left[\tfrac{1}{6}\alpha^{-3} + 2\alpha^{-1} + \tfrac{1}{48}(\pi\alpha)^3\right](4K+5)^{-1/2} + \left[\tfrac{1}{72}\alpha^{-6} + \tfrac{1}{3}\alpha^{-4} + \tfrac{7}{4}\alpha^{-2} + \tfrac{1}{288}\pi^3 - 1 + \left(\tfrac{1}{24}\pi - \tfrac{1}{16}\right)(\pi\alpha)^2 + \tfrac{1}{4608}(\pi\alpha)^6\right](4K+5)^{-1} + O\left(K^{-3/2}\right)\right\}, \quad (A50)$$

$$-(4K+5)^{-1/2}\,2^{1/2}\sum_{k=0}^{K} V_{K,k}\left(U^{-1}\right)_{k,K} = -(4K+5)^{-1/2}\,2^{-1/2}\alpha^{-1}V_{K,K}\left(U^{-1}\right)_{K,K}\left[1 + O\left(K^{-1/2}\right)\right] = 4(\pi\alpha)^{-1}(4K+5)^{-3/2}\left[1 + O\left(K^{-1/2}\right)\right], \quad (A51)$$

$$-U_{K,K+1}\sum_{k=0}^{K}\sum_{\ell=K+1}^{\infty}\left(U^{-1}\right)_{k,K}V_{k,\ell}\left(\bar{c}_{K+1}^{(\mathrm{TP})}c_\ell^{(\mathrm{TP})} + \bar{c}_\ell^{(\mathrm{TP})}c_{K+1}^{(\mathrm{TP})}\right)$$

$$= 8\pi^{-1}(4K+5)^{-1}\exp\left[-2\alpha^{-1}(4K+5)^{1/2}\right]\left[1 + O\left(K^{-1/2}\right)\right], \quad (A52)$$

$$-U_{K,K+1}\sum_{k=0}^{K}\sum_{\ell=K+1}^{\infty}\left(U^{-1}\right)_{k,K}V_{k,\ell}\left(\bar{c}_{K+1}^{(\mathrm{sing})}c_\ell^{(\mathrm{TP})} + \bar{c}_\ell^{(\mathrm{sing})}c_{K+1}^{(\mathrm{TP})} + \bar{c}_{K+1}^{(\mathrm{TP})}c_\ell^{(\mathrm{sing})} + \bar{c}_\ell^{(\mathrm{TP})}c_{K+1}^{(\mathrm{sing})}\right)$$

$$= 2^{5/2}\pi^{-3/2}\alpha\zeta\left(2, \tfrac{1}{2}\alpha + \tfrac{1}{2}\right)(-1)^{K+1}(4K+5)^{-1/2}\exp\left[-\left(\tfrac{1}{2}\pi\alpha + \alpha^{-1}\right)(4K+5)^{1/2}\right]\left[1 + O\left(K^{-1/2}\right)\right]. \quad (A53)$$

Evaluation of the first numerator term in (2.32) from (A37)–(A45) and the second numerator term from (A47)–(A53) shows that best approximation in L^2 again yields the result (4.12)–(4.15) for the error $\tilde{E}^{(\mathrm{RR};K)} - E$. The pieces that combine to yield the contributions that come from (A28)–(A30) when best approximation in H^1 is used can be identified with the aid of the identity

$$\sum_{k=K+1}^{\infty}\sum_{\ell=K+1}^{\infty}\bar{c}_k T_{k,\ell} c_\ell + \tfrac{1}{2}\sum_{k=K+1}^{\infty}|c_k|^2 - |U_{K,K+1}c_{K+1}|^2 = \sum_{k=K+1}^{\infty}|\hat{c}_k|^2, \quad (A54)$$

which can be derived from (2.10), (2.12), (2.18), and (2.20).

APPENDIX B: DETAILS FOR THE HYDROGEN ATOM

The computations begin with the kinetic and potential energy matrix elements, which are defined by

$$T_{k,\ell} = \int_0^\infty \left[\frac{d}{dz}e_{2k+1}(\alpha; z)\right]\left[\frac{d}{dz}e_{2\ell+1}(\alpha; z)\right] dz, \quad (B1)$$

$$V_{k,\ell} = -2\int_0^\infty e_{2k+1}(\alpha; z)\,\frac{1}{z}\,e_{2\ell+1}(\alpha; z)\,dz. \quad (B2)$$

The kinetic energy matrix elements $T_{k,\ell}$ are given explicitly by

$$T_{k,\ell} = \tfrac{1}{4}\alpha^2 \left\{ - \left[(2\ell+3)(2\ell+2)\right]^{1/2} \delta_{k,\ell+1} + (4\ell+3)\,\delta_{k,\ell} - \left[2\ell+1\,(2\ell)\right]^{1/2} \delta_{k,\ell-1} \right\}. \quad \text{(B3)}$$

There does not appear to be any simple formula for the potential energy matrix elements $V_{k,\ell}$. However, an asymptotic formula for $V_{k,\ell}$ is given in [1], Eq. (5.43). It is

$$V_{k,\ell} = -\alpha\pi^{-1}(-1)^{k+\ell}(k\ell)^{-1/4} \times \left\{ 2\ln\left(\sqrt{k}+\sqrt{\ell}\right) - \Psi\left(|k-\ell|+\tfrac{1}{2}\right) + O\left[1/\min(k,\ell)\right] \right\}. \quad \text{(B4)}$$

The evaluation of the error when the best approximation in H^1 is used as a trial function begins with the construction of asymptotic formulas for the elements $U_{k,\ell}$ of the upper triangular matrix that appears in (2.19). Since $T_{k,\ell}$ is tridiagonal, the computation parallels that done for the $\cosh^{-2}$ potential; the result is

$$U_{k,k} = \tfrac{1}{4}\sqrt{2}\alpha\,(4k+3)^{1/2} + \tfrac{1}{2}|\beta| + \tfrac{1}{8}\sqrt{2}\alpha^{-1}\left(\alpha^2+2\beta^2\right)(4k+3)^{-1/2} - \tfrac{1}{4}|\beta|\,(4k+3)^{-1} - \tfrac{1}{32}\sqrt{2}\alpha^{-3}\left(\alpha^2+2\beta^2\right)^2 \times (4k+3)^{-3/2} + O\left(k^{-2}\right), \quad \text{(B5)}$$

$$U_{k,k+1} = -\tfrac{1}{4}\sqrt{2}\alpha\,(4k+3)^{1/2} + \tfrac{1}{2}|\beta| - \tfrac{1}{8}\sqrt{2}\alpha^{-1}\left(3\alpha^2+2\beta^2\right)(4k+3)^{-1/2} + \tfrac{1}{4}|\beta|\,(4k+3)^{-1} + \tfrac{1}{32}\sqrt{2}\alpha^{-3}\left(3\alpha^2+2\beta^2\right)^2 \times (4k+3)^{-3/2} + O\left(k^{-2}\right). \quad \text{(B6)}$$

The derivation of the asymptotic formulas for the elements $\left(U^{-1}\right)_{k,\ell}$ of the upper triangular matrix inverse to $U_{k,\ell}$, which are needed for the computation of asymptotic formulas for the potential energy matrix elements $\langle\eta_k|V|\eta_\ell\rangle$ and the Gram matrix elements $\langle\eta_k|\eta_\ell\rangle$, also parallels that done for the $\cosh^{-2}$ potential; the result is

$$\left(U^{-1}\right)_{k,\ell} = 2^{3/2}\alpha^{-1}\left[(4\ell+3)(4k+3)\right]^{-1/4}\exp\left\{\alpha^{-1}2^{1/2}|\beta|\left[(4k+3)^{1/2}-(4\ell+3)^{1/2}\right]\right\} \times \left\{1+\tfrac{7}{6}\left(\alpha^{-1}2^{1/2}|\beta|\right)^3\left[(4k+3)^{-1/2}-(4\ell+3)^{-1/2}\right] - \alpha^{-1}2^{1/2}|\beta|\,(4\ell+3)^{-1/2} + O\left(k^{-1}\right)\right\}. \quad \text{(B7)}$$

The desired asymptotic formulas for matrix elements with respect to the $|\eta_k\rangle$ can be calculated from (2.2), (2.7), (B4), and (B7) with the aid of the Euler-Maclaurin sum formula and summation by parts. For $\langle\eta_k|\eta_\ell\rangle$, the sums can be evaluated via analogs of the sum formulas (A11) and (A15); the result is

$$\langle\eta_k|\eta_\ell\rangle = 2n^2(\alpha n)^{-1}\left[(4k+3)(4\ell+3)\right]^{-1/4}\exp\left[-(n\alpha)^{-1}\left|(4k+3)^{1/2}-(4\ell+3)^{1/2}\right|\right] \times \left\{1-\left[(n\alpha)^{-1}+\tfrac{7}{6}(n\alpha)^{-3}\right] \times \left|(4k+3)^{-1/2}-(4\ell+3)^{-1/2}\right| + O\left(k^{-1}\right)+O\left(\ell^{-1}\right)\right\}. \quad \text{(B8)}$$

The derivation of the formula for $\langle\eta_k|V|\eta_\ell\rangle$ is somewhat more difficult. The term in (B4) that involves $\ln(\sqrt{k}+\sqrt{\ell})$ can be evaluated with the aid of (A14), but the function $\Psi\left(|k-\ell|+\frac{1}{2}\right)$ varies too rapidly near $k=\ell$ to permit using (A14) for the asymptotic evaluation of the sums for this part. The function $\Psi\left(|k-\ell|+\frac{1}{2}\right)$ must be included in the $\Delta_j g(j)$ that is summed when the summation by parts formula (A13) is used. The formulas needed to perform the repeated summations can be conveniently summarized by making the definitions

$$g_1(z;j) = (-1)^j\,\Psi(z+j), \quad \text{(B9)}$$

$$g_2(z;j) = -\tfrac{1}{2}(-1)^j\left\{\Psi\left[\tfrac{1}{2}(z+j)\right]+\ln(2)\right\}, \quad \text{(B10)}$$

$$g_3(z;j) = \tfrac{1}{4}(-1)^j\left\{(z+j-1)\,\Psi\left[\tfrac{1}{2}(z+j+1)\right]-(z+j-2)\,\Psi\left[\tfrac{1}{2}(z+j)\right]-1+\ln(2)\right\}, \quad \text{(B11)}$$

$$g_4(z;j) = -\tfrac{1}{16}(-1)^j\left\{(z+j-2)(z+j)\,\Psi\left[\tfrac{1}{2}(z+j+2)\right]-2(z+j-3)(z+j-1)\,\Psi\left[\tfrac{1}{2}(z+j+1)\right] + (z+j-4)(z+j-2)\,\Psi\left[\tfrac{1}{2}(z+j)\right]-3+2\ln(2)\right\}, \quad \text{(B12)}$$

$$h_1(z;j) = (-1)^j\,\Psi(z-j), \quad \text{(B13)}$$

$$h_2(z;j) = -\tfrac{1}{2}(-1)^j\left\{\Psi\left[\tfrac{1}{2}(z-j+1)\right]+\ln(2)\right\}, \quad \text{(B14)}$$

$$h_3(z;j) = \tfrac{1}{4}(-1)^j\left\{(z-j+1)\,\Psi\left[\tfrac{1}{2}(z-j+3)\right]-(z-j)\,\Psi\left[\tfrac{1}{2}(z-j+2)\right]-1+\ln(2)\right\}, \quad \text{(B15)}$$

$$h_4(z;j) = -\tfrac{1}{16}(-1)^j\left\{(z-j+1)(z-j+3)\,\Psi\left[\tfrac{1}{2}(z-j+5)\right]-2(z-j)(z-j+2)\,\Psi\left[\tfrac{1}{2}(z-j+4)\right] + (z-j-1)(z-j+1)\,\Psi\left[\tfrac{1}{2}(z-j+3)\right]-3+2\ln(2)\right\}. \quad \text{(B16)}$$

Identities for the Ψ function can be used to show that

$$\Delta_j g_{k+1}(z;j) = g_k(z;j)\,, \tag{B17}$$

$$\Delta_j h_{k+1}(z;j) = h_k(z;j)\,. \tag{B18}$$

Using the summation by parts formula (A13) twice, differencing $h(\ell)$, and summing $(-1)^{\ell+1}\Psi\left(|\ell-\ell'|+\frac{1}{2}\right)$ with the aid of (B9)–(B18) yields the result

$$\begin{aligned}\sum_{\ell=0}^{k}&(-1)^{\ell+1}\Psi\left(|\ell-\ell'|+\tfrac{1}{2}\right)h(\ell)\\ &\approx \tfrac{1}{2}\pi(-1)^{\ell'}h(\ell')+\tfrac{1}{2}(-1)^{k+1}\left\{\Psi\left[\tfrac{1}{2}(k-\ell')+\tfrac{3}{4}\right]+\ln(2)\right\}h(k+1)\\ &\quad+\tfrac{1}{4}(-1)^{k+1}\left\{\left(k-\ell'+\tfrac{1}{2}\right)\Psi\left[\tfrac{1}{2}(k-\ell')+\tfrac{5}{4}\right]-\left(k-\ell'+\tfrac{3}{2}\right)\Psi\left[\tfrac{1}{2}(k-\ell')+\tfrac{7}{4}\right]+1-\ln(2)\right\}\Delta_k h(k)\,,\end{aligned} \tag{B19}$$

which is used with the choice

$$h(\ell) = (4\ell+3)^{-1/4}\left(U^{-1}\right)_{\ell,k} \tag{B20}$$

to perform the needed sum over ℓ when $\ell' \le k$. The asymptotic evaluation of the sum over ℓ' that involves the Ψ function is similar. The result is

$$\langle\eta_k|V|\eta_{k'}\rangle = \hat{V}^{(a)}_{k,k'}+\hat{V}^{(b)}_{k,k'}, \tag{B21}$$

where

$$\begin{aligned}\hat{V}^{(a)}_{k,k'} &= -2n\,(4k_>+3)^{-1/4}(4k_<+3)^{-3/4}\exp\left\{-(\alpha n)^{-1}\left[(4k_>+3)^{1/2}-(4k_<+3)^{1/2}\right]\right\}\\ &\quad\times\left\{1+\tfrac{1}{2}\alpha n\,(4k_<+3)^{-1/2}+\left[\tfrac{7}{6}(\alpha n)^{-3}+(\alpha n)^{-1}\right]\left[(4k_<+3)^{-1/2}-(4k_>+3)^{-1/2}\right]+O\left(k_<^{-1}\right)\right\},\end{aligned} \tag{B22}$$

$$\begin{aligned}\hat{V}^{(b)}_{k,k'} &= -4(\pi\alpha)^{-1}(-1)^{k+k'}\left[(4k+3)(4k'+3)\right]^{-3/4}\left\{2\ln\left[(4k+3)^{1/2}+(4k'+3)^{1/2}\right]\right.\\ &\quad-2\ln(2)-\Psi\left(|k-k'|+\tfrac{1}{2}\right)+f(|k-k'|)\\ &\quad\left.+(\alpha n)^{-1}\left[(4k_<+3)^{-1/2}-(4k_>+3)^{-1/2}\right]g(|k-k'|)+O\left(k_<^{-1}\right)\right\}.\end{aligned} \tag{B23}$$

Here $k_<$ is the smaller of the pair k, k' and $k_>$ is the larger of the pair k, k'. The functions f and g are defined by

$$f(x) = x\left[\Psi\left(\tfrac{1}{2}x-\tfrac{1}{4}\right)-\Psi\left(\tfrac{1}{2}x+\tfrac{1}{4}\right)\right]+1+\left(x-\tfrac{1}{2}\right)^{-1}, \tag{B24}$$

$$g(x) = \left(x^2-\tfrac{1}{4}\right)\left[\Psi\left(\tfrac{1}{2}x-\tfrac{1}{4}\right)-\Psi\left(\tfrac{1}{2}x+\tfrac{1}{4}\right)\right]+x+1. \tag{B25}$$

Both $f(x)$ and $g(x)$ are bounded for x a non-negative integer. For x large and positive, $f(x) = O\left(x^{-2}\right)$ and $g(x) = O\left(x^{-1}\right)$.

The singularity and the turning point contributions to $\hat{c}_k$ can be calculated by setting β^2 equal to $-E_n = 1/(2n^2)$ and using $\hat{c}_k = U_{k,k}c_k + U_{k,k+1}c_{k+1}$. The results are

$$\hat{c}_k^{(\text{cusp})} = 2^{5/2}\pi^{-1/2}(n\alpha)^{-3/2}(-1)^k(4k+3)^{-5/4}\left\{1-\left[\tfrac{5}{2}+\tfrac{2}{3}\alpha^{-2}+\tfrac{5}{6}(n\alpha)^{-2}\right](4k+3)^{-1}+O\left(k^{-3/2}\right)\right\}, \tag{B26}$$

$$\begin{aligned}\hat{c}_k^{(\text{TP})} &= \alpha^{1/2}(4k+3)^{-1/4}\left\{\phi_n^{(0)}\left(x_{2k+1}^{(0)}\right)+\left[\alpha^{-1}\phi_n^{(1)}\left(x_{2k+1}^{(0)}\right)+\tfrac{1}{6}\alpha^{-3}\phi_n^{(3)}\left(x_{2k+1}^{(0)}\right)\right](4k+3)^{-1/2}\right.\\ &\quad+\left[-\tfrac{1}{2}\phi_n^{(0)}\left(x_{2k+1}^{(0)}\right)-\tfrac{1}{2}\alpha^{-1}(n\alpha)^{-1}\phi_n^{(1)}\left(x_{2k+1}^{(0)}\right)+\tfrac{1}{4}\alpha^{-2}\phi_n^{(2)}\left(x_{2k+1}^{(0)}\right)+\tfrac{1}{6}\alpha^{-4}\phi_n^{(4)}\left(x_{2k+1}^{(0)}\right)\right.\\ &\quad\left.\left.+\tfrac{1}{72}\alpha^{-6}\phi_n^{(6)}\left(x_{2k+1}^{(0)}\right)\right](4k+3)^{-1}+O\left[\phi_n^{(0)}\left(x_{2k+1}^{(0)}\right)k^{-3/2}\right]\right\},\end{aligned} \tag{B27}$$

where the $\phi_n^{(j)}(x)$ are defined in (5.16) above. The various contributions to $\langle\delta\psi^{(H^1;K)}|H-EI|\delta\psi^{(H^1;K)}\rangle$ can now be calculated. The easiest are the contributions to $\langle\delta\psi^{(H^1;K)}|T+\beta^2 I|\delta\psi^{(H^1;K)}\rangle$, which are just $\sum_{k=K+1}^{\infty}|\hat{c}_k|^2$ as a consequence of (2.8) and (2.11). Performing the sums over k with the aid of the Euler-MacLaurin sum formula and integration by parts yields

$$\sum_{k=K+1}^{\infty} |\hat{c}_k^{(\mathrm{cusp})}|^2 = \tfrac{16}{3}\pi^{-1}(n\alpha)^{-3}(4K+7)^{-3/2}\left\{1-\left[\tfrac{4}{5}\alpha^{-2}+(n\alpha)^{-2}\right](4K+7)^{-1}+O\left(K^{-3/2}\right)\right\}, \tag{B28}$$

$$\begin{aligned}\sum_{k=K+1}^{\infty} |\hat{c}_k^{(\mathrm{TP})}|^2 = {}& \tfrac{1}{2}\alpha^2 \int_{x_{2K+3}^{(0)}}^{\infty} \left[\phi_n^{(0)}(x)\right]^2 dx \\ & -\tfrac{1}{6}\alpha^{-1}\left\{\phi_n^{(0)}\left(x_{2K+3}^{(0)}\right)\phi_n^{(2)}\left(x_{2K+3}^{(0)}\right)-\tfrac{1}{2}\left[\phi_n^{(1)}\left(x_{2K+3}^{(0)}\right)\right]^2\right\}(4K+7)^{-1/2} \\ & +\left\{\tfrac{1}{4}n^{-1}\left[\phi_n^{(0)}\left(x_{2K+3}^{(0)}\right)\right]^2+\tfrac{1}{4}\phi_n^{(0)}\left(x_{2K+3}^{(0)}\right)\phi_n^{(1)}\left(x_{2K+3}^{(0)}\right)\right. \\ & -\tfrac{1}{72}\alpha^{-4}\left[\phi_n^{(0)}\left(x_{2K+3}^{(0)}\right)\phi_n^{(5)}\left(x_{2K+3}^{(0)}\right)-\phi_n^{(1)}\left(x_{2K+3}^{(0)}\right)\phi_n^{(4)}\left(x_{2K+3}^{(0)}\right)\right. \\ & \left.\left.+\phi_n^{(2)}\left(x_{2K+3}^{(0)}\right)\phi_n^{(3)}\left(x_{2K+3}^{(0)}\right)\right]\right\}(4K+7)^{-1}+O\left\{K^{-3/2}\left[\phi_n^{(0)}\left(x_{2K+3}^{(0)}\right)\right]^2\right\},\end{aligned} \tag{B29}$$

$$\begin{aligned}&\sum_{k=K+1}^{\infty}\left[\bar{\hat{c}}_k^{(\mathrm{cusp})}\hat{c}_k^{(\mathrm{TP})}+\bar{\hat{c}}_k^{(\mathrm{TP})}\hat{c}_k^{(\mathrm{cusp})}\right] \\ &\quad = 4\left(\frac{2\alpha}{\pi}\right)^{1/2}(n\alpha)^{-3/2}(-1)^{K+1}(4K+7)^{-3/2} \\ &\qquad \times\left\{\phi_n^{(0)}\left(x_{2K+3}^{(0)}\right)+\tfrac{1}{6}\alpha^{-3}\phi_n^{(3)}\left(x_{2K+3}^{(0)}\right)(4K+7)^{-1/2}+O\left[K^{-1}\phi_n^{(0)}\left(x_{2K+3}^{(0)}\right)\right]\right\}.\end{aligned} \tag{B30}$$

The contributions to $\langle\delta\psi^{(H^1;K)}|V|\delta\psi^{(H^1;K)}\rangle$ are

$$\sum_{k=K+1}^{\infty}\sum_{\ell=K+1}^{\infty}\bar{\hat{c}}_k^{(\mathrm{cusp})}\langle\eta_k|V|\eta_\ell\rangle\hat{c}_\ell^{(\mathrm{cusp})} = -16\pi^{-2}n(n\alpha)^{-4}(4K+7)^{-2}\left[1+O\left(K^{-1}\right)\right], \tag{B31}$$

$$\begin{aligned}&\sum_{k=K+1}^{\infty}\sum_{\ell=K+1}^{\infty}\bar{\hat{c}}_k^{(\mathrm{TP})}\langle\eta_k|V|\eta_\ell\rangle\hat{c}_\ell^{(\mathrm{TP})} \\ &\quad = -n\alpha\left[1+\tfrac{1}{2}n\alpha(4K+7)^{-1/2}\right]\int_{x_{2K+3}^{(0)}}^{\infty} x^{-1}\phi_n^{(0)}(x)\,\psi_n(x)\,dx \\ &\qquad -\tfrac{1}{6}\left\{\left[\phi_n^{(0)}\left(x_{2K+3}^{(0)}\right)\right]^2-\left[\alpha^{-2}(n\alpha)\phi_n^{(2)}\left(x_{2K+3}^{(0)}\right)-\alpha^{-1}\phi_n^{(1)}\left(x_{2K+3}^{(0)}\right)+(n\alpha)^{-1}\phi_n^{(0)}\left(x_{2K+3}^{(0)}\right)\right]\right. \\ &\qquad \left.\times\psi_n\left(x_{2K+3}^{(0)}\right)\right\}(4K+7)^{-1}+O\left\{K^{-3/2}\left[\phi_n^{(0)}\left(x_{2K+3}^{(0)}\right)\right]^2\right\},\end{aligned} \tag{B32}$$

$$\begin{aligned}&\sum_{k=K+1}^{\infty}\sum_{\ell=K+1}^{\infty}\left[\bar{\hat{c}}_k^{(\mathrm{cusp})}\hat{c}_\ell^{(\mathrm{TP})}+\bar{\hat{c}}_k^{(\mathrm{TP})}\hat{c}_\ell^{(\mathrm{cusp})}\right]\langle\eta_k|V|\eta_\ell\rangle \\ &\quad = -4\left(\frac{2\alpha}{\pi}\right)^{1/2}(n\alpha)^{-3/2}(-1)^{K+1}(4K+7)^{-2}\left\{n\psi_n\left(x_{2K+3}^{(0)}\right)+\left(\frac{2}{\pi\alpha}\right)\phi_n^{(0)}\left(x_{2K+3}^{(0)}\right)\right. \\ &\qquad \left.+O\left[K^{-1/2}\phi_n^{(0)}\left(x_{2K+3}^{(0)}\right)\right]\right\}.\end{aligned} \tag{B33}$$

It is straightforward to show that the denominator of the error formula (2.32) is given by

$$\langle\tilde{\psi}^{(H^1;K)}|\tilde{\psi}^{(H^1;K)}\rangle = 1-\sum_{k=0}^{K}\sum_{\ell=K+1}^{\infty}\left[\bar{\tilde{c}}_k\langle\eta_k|\eta_\ell\rangle\hat{c}_\ell+\bar{\hat{c}}_\ell\langle\eta_\ell|\eta_k\rangle\tilde{c}_k\right]-\sum_{k=K+1}^{\infty}\sum_{\ell=K+1}^{\infty}\bar{\hat{c}}_k\langle\eta_k|\eta_\ell\rangle\hat{c}_\ell. \tag{B34}$$

The pieces needed for the evaluation of (B34) are

$$\sum_{k=K+1}^{\infty}\sum_{\ell=K+1}^{\infty} \bar{c}_k^{(\mathrm{cusp})}\hat{c}_\ell^{(\mathrm{cusp})}\langle\eta_k|\eta_\ell\rangle = 32\,(5\pi)^{-1}\,\alpha^{-2}\,(n\alpha)^{-3}\,(4K+7)^{-5/2}\left[1+O\left(K^{-1/2}\right)\right], \tag{B35}$$

$$\sum_{k=K+1}^{\infty}\sum_{\ell=K+1}^{\infty} \bar{c}_k^{(\mathrm{TP})}\langle\eta_k|\eta_\ell\rangle\hat{c}_\ell^{(\mathrm{TP})} = n\alpha\int_{x_{2K+3}^{(0)}}^{\infty}\phi_n^{(0)}(x)\,\psi_n(x)\,dx\left[1+O\left(K^{-1/2}\right)\right], \tag{B36}$$

$$\sum_{k=K+1}^{\infty}\sum_{\ell=K+1}^{\infty}\left[\bar{c}_k^{(\mathrm{cusp})}\langle\eta_k|\eta_\ell\rangle\hat{c}_\ell^{(\mathrm{TP})}+\bar{c}_k^{(\mathrm{TP})}\langle\eta_k|\eta_\ell\rangle\hat{c}_\ell^{(\mathrm{cusp})}\right]$$

$$= 2^{5/2}\pi^{-1/2}\alpha^{-3/2}\,(n\alpha)^{-1/2}\,(-1)^{K+1}\,(4K+7)^{-3/2}\,\psi_n\left(x_{2K+3}^{(0)}\right)\left[1+O\left(K^{-1/2}\right)\right], \tag{B37}$$

$$\sum_{k=0}^{K}\sum_{\ell=K+1}^{\infty}\left[\bar{c}_k^{(\mathrm{cusp})}\langle\eta_k|\eta_\ell\rangle\hat{c}_\ell^{(\mathrm{cusp})}+\bar{c}_\ell^{(\mathrm{cusp})}\langle\eta_\ell|\eta_k\rangle\hat{c}_k^{(\mathrm{cusp})}\right] = -32\pi^{-1}\alpha^{-2}\,(n\alpha)^{-2}\,(4K+7)^{-3}\left[1+O\left(K^{-1/2}\right)\right], \tag{B38}$$

$$\sum_{k=0}^{K}\sum_{\ell=K+1}^{\infty}\left[\bar{c}_k^{(\mathrm{TP})}\langle\eta_k|\eta_\ell\rangle\hat{c}_\ell^{(\mathrm{TP})}+\bar{c}_\ell^{(\mathrm{TP})}\langle\eta_\ell|\eta_k\rangle\hat{c}_k^{(\mathrm{TP})}\right]$$

$$= -2\,(n+1)^{-1}\,n^{-1/2}x_{2K+3}^{(0)}\exp\left(-x_{2K+3}^{(0)}/n\right)L_n^{(1)}\left(2x_{2K+3}^{(0)}/n\right)\psi_n\left(x_{2K+3}^{(0)}\right)\left[1+O\left(K^{-1/2}\right)\right], \tag{B39}$$

$$\sum_{k=0}^{K}\sum_{\ell=K+1}^{\infty}\left[\bar{c}_k^{(\mathrm{cusp})}\langle\eta_k|\eta_\ell\rangle\hat{c}_\ell^{(\mathrm{TP})}+\bar{c}_\ell^{(\mathrm{cusp})}\langle\eta_\ell|\eta_k\rangle\hat{c}_k^{(\mathrm{TP})}+\bar{c}_k^{(\mathrm{TP})}\langle\eta_k|\eta_\ell\rangle\hat{c}_\ell^{(\mathrm{cusp})}+\bar{c}_\ell^{(\mathrm{TP})}\langle\eta_\ell|\eta_k\rangle\hat{c}_k^{(\mathrm{cusp})}\right]$$

$$= -2^{5/2}\pi^{-1/2}\alpha^{-3/2}\,(n\alpha)^{-1/2}\,(-1)^{K+1}\,(4K+7)^{-3/2}$$

$$\times\left[2\,(n+1)^{-1}\,n^{-3/2}x_{2K+3}^{(0)}\exp\left(-x_{2K+3}^{(0)}/n\right)L_n^{(1)}\left(2x_{2K+3}^{(0)}/n\right)\right.$$

$$\left.+\psi_n\left(x_{2K+3}^{(0)}\right)\right]\left[1+O\left(K^{-1/2}\right)\right]. \tag{B40}$$

The results (5.13)–(5.15) for best approximation in H^1 can now be assembled by adding up the contributions to $\langle\delta\psi^{(H^1;K)}|\,(H-EI)\,|\delta\psi^{(H^1;K)}\rangle$ from (B28)–(B33). Formulas (B34)–(B40) can be used to show that the denominator of the error formula (2.32) is 1 to the order to which the calculation has been carried. The integrals that appear in (5.14) can be evaluated with the aid of the formulas

$$\int_s^{\infty}\exp(-t)\left[L_n^{(0)}(t)\right]^2 dt$$

$$= \left\{1+\sum_{m=0}^{n-1}\left[\frac{sL_m^{(1)}(s)}{m+1}\right]^2\right\}\exp(-s), \tag{B41}$$

$$\int_s^{\infty}\exp(-t)\,L_{n-1}^{(1)}(t)\,L_n^{(0)}(t)\,dt$$

$$= -s\sum_{m=0}^{n-1}\frac{L_m^{(0)}(s)\,L_m^{(1)}(s)}{m+1}\exp(-s). \tag{B42}$$

APPENDIX C: DETAILS FOR THE x^4 ANHARMONIC OSCILLATOR

This appendix records the large z asymptotic expansion of the wave function $\psi(z)$ and presents some of the details of the saddle point approximation to the expansion coefficient c_k.

The asymptotic expansion of $\psi(z)$ will be considered first. Adopt the convention $b_\ell = 0, \ell < 0$. Let $b_0 = 1$ and compute coefficients b_ℓ for $\ell > 0$ recursively from

$$b_\ell = -\frac{1}{2\lambda^{1/2}\ell}\left[\left(E + \frac{1}{4\lambda}\right) b_{\ell-1} + \lambda^{-1/2}(\ell-1) b_{\ell-2} + (\ell-1)(\ell-2) b_{\ell-3}\right]. \tag{C1}$$

The first few coefficients are given explicitly by

$$b_0 = 1, \tag{C2}$$

$$b_1 = -\frac{4\lambda E + 1}{8\lambda^{3/2}}, \tag{C3}$$

$$b_2 = \frac{16\lambda^2(E-2) + 8\lambda E + 1}{128\lambda^3}. \tag{C4}$$

Define $B_m(z)$ by

$$B_m(z) = \sum_{\ell=0}^{m} b_\ell z^{-\ell-1}. \tag{C5}$$

Then the large z behavior of $\psi(z)$ is given by

$$\psi(z) = C_+ \exp\left(-\tfrac{1}{3}\lambda^{1/2}z^3 - \tfrac{1}{2}\lambda^{-1/2}z\right)\left[B_m(z) + O\left(z^{-m-2}\right)\right] \quad \text{for } z\to\infty \text{ with } -\tfrac{1}{2}\pi < \arg(z) < \tfrac{1}{2}\pi, \tag{C6}$$

$$\psi(z) = C_- \exp\left(\tfrac{1}{3}\lambda^{1/2}z^3 + \tfrac{1}{2}\lambda^{-1/2}z\right)\left[B_m(-z) + O\left(z^{-m-2}\right)\right] \quad \text{for } z\to\infty \text{ with } \tfrac{1}{2}\pi < \arg(z) < \tfrac{3}{2}\pi, \tag{C7}$$

$$\begin{aligned}\psi(z) = {} & C_+ \exp\left(-\tfrac{1}{3}\lambda^{1/2}z^3 - \tfrac{1}{2}\lambda^{-1/2}z\right)\left[B_m(z) + O\left(z^{-m-2}\right)\right] \\ & + C_- \exp\left(\tfrac{1}{3}\lambda^{1/2}z^3 + \tfrac{1}{2}\lambda^{-1/2}z\right)\left[B_m(-z) + O\left(z^{-m-2}\right)\right] \\ & \text{for } z\to\infty \text{ with } \tfrac{1}{6}\pi < \arg(z) < \tfrac{5}{6}\pi \text{ and for } z\to\infty \text{ with } -\tfrac{5}{6}\pi < \arg(z) < -\tfrac{1}{6}\pi.\end{aligned} \tag{C8}$$

C_+ and C_- are determined by the normalization condition imposed on ψ. For even parity states, $C_- = C_+$. For odd parity states, $C_- = -C_+$. The apparent inconsistency between (C6) and (C8) in a domain such as $\frac{1}{6}\pi < \arg(z) < \frac{1}{2}\pi$ where both (C6) and (C8) are valid is resolved when one notes that the terms in (C8) that are not present in (C6) are exponentially small for z tending to infinity in $\frac{1}{6}\pi < \arg(z) < \frac{1}{2}\pi$. This is an example of the Stokes phenomenon [37], which occurs here because an entire function of z^2 is being approximated by multiple valued functions of z^2 ($z = \sqrt{z^2}$ is a multiple valued function of z^2). For the ground state with $\lambda = 1$,

$$C_+ = C_- = 2.237\,250\,255\,9\ldots . \tag{C9}$$

The value of $C_- = C_+$ given in (C9) was obtained by using a package for the numerical solution of systems of ordinary differential equations to obtain $\psi(0)/C_+$ by integrating the Schrödinger equation [with E given by (6.1)] from a point x_0 on the positive real axis in to the origin. x_0 is chosen sufficiently large so that the asymptotic expansion (C6) gives initial values of $\psi(x_0)/C_+$ and $\psi'(x_0)/C_+$ to machine accuracy. C_+ is then chosen to make $\psi(0)$ agree with the value of $\psi(0)$ obtained from the variational wave function that gives the energy (6.1).

The saddle point evaluation of the integrals (6.5) begins by writing the integrands in the form $g(z)\exp[w(z)]$, where $\exp[w(z)]$ consists of the exponential factors from (3.10) and (C6) or (C7) as appropriate, and $g(z)$ is the rest of the integrand. For the integrands of (6.5) with z in the right half plane,

$$w(z) = -\tfrac{1}{3}\lambda^{1/2}z^3 - \tfrac{1}{2}\lambda^{-1/2}z + (2k+1)\xi(t), \tag{C10}$$

where $\xi(t)$ is given by (3.11) and t by (3.12). For z in the left half plane, the exponential factor from (C6) would be replaced by the exponential factor from (C7). The derivative of $w(z)$ is

$$dw(z)/dz = -\lambda^{1/2}z^2 - \tfrac{1}{2}\lambda^{-1/2} + \alpha\left[\alpha^2 z^2 - (2k+1)\right]^{1/2}. \tag{C11}$$

The saddle points in the right half plane occur at the zeros z_+ and z_- of $dw(z)/dz$, which are given by (6.9)–(6.13) above. Because the asymptotic expansion (3.10) applied to $e_k^{(+)}(\alpha; z)$ differs from the asymptotic expansion (3.10) applied to $e_k^{(-)}(\alpha; z)$ only in sign, the integrals $c_k^{(+)}$ and $c_k^{(-)}$ can be combined after the asymptotic approximation (3.10) has been made. By symmetry, the contribution of the integration contours in the left half plane is the same as the contribution from the integration contours in the right half plane. Hence

$$c_k = \int_C dz\, g(z)\exp[w(z)]\left[1 + O\left(k^{-1}\right)\right], \tag{C12}$$

where $w(z)$ is given by (C10) and $g(z)$ is given by

$$g(z) = -2iC_+ (2\pi)^{-1/2} (2k+1)^{-1/4} \times \alpha^{1/2} (t^2-1)^{-1/4} B_2(z), \quad \text{(C13)}$$

with t again given by (3.12). The integration contours in the complex plane used for (C12) in the two cases $k \le k_c$ and $k > k_c$ are shown in Figs. 3 and 4. The contours for the first case change smoothly into the contours for the second as k moves through k_c. The contributions from the pieces of the contour that run from $-\infty$ to $-z_-$ and from z_- to $+\infty$ on the real axis are negligible when $k < k_c$. The $O(k^{-1})$ error estimate in (C12) and the decision to use $B_2(z)$ in $g(z)$ result from assuming $\alpha = O(k^{1/6})$, which in turn implies $z = O(k^{1/3})$ for z near z_+ or z_-. Only the leading term in (3.10) is taken. Clearly $\alpha = O(k^{1/6})$ for k near k_c.

The formulas for asymptotic expansions of integrals with two nearby saddle points that are used (see [22], pp. 369–379, or [23], pp. 366–372) are

$$w(z) = \rho + \gamma^2 s - \tfrac{1}{3}s^3, \quad \text{(C14)}$$

$$\tfrac{4}{3}\gamma^3 = w(z_+) - w(z_-), \quad \text{(C15)}$$

$$\rho = \tfrac{1}{2}[w(z_+) + w(z_-)], \quad \text{(C16)}$$

$$\left[\frac{dz}{ds}\right]_{s=\pm\gamma} = \left(\frac{2\gamma}{\delta}\right)^{1/2} \left[\mp\frac{1}{\delta}\left(\frac{d^2w}{dz^2}\right)_{z=z_\pm}\right]^{-1/2}, \quad \text{(C17)}$$

$$G_0(s) = g[z(s)]\frac{dz}{ds}, \quad \text{(C18)}$$

$$a_0 = \tfrac{1}{2}[G_0(s_+) + G_0(s_-)], \quad \text{(C19)}$$

$$a_1 = \frac{1}{2\gamma}[G_0(s_+) - G_0(s_-)], \quad \text{(C20)}$$

and (6.15) above. Equations (C14)–(C18) are Eqs. (9.2.6), (9.2.9), (9.2.10), (9.2.11), and (9.2.19) of [22] in a simplified notation and with t replaced by s. Equations (C19) and (C20) are Eqs. (9.2.21) of [22]. Equation (6.15) is Eq. (9.2.29) of [22] with λ replaced by 1. The basic idea is that the change of variables from z to s given implicitly by (C14), together with expansions of $G_0(s)$ about the saddle points, are used to bring (C12) to forms that can be recognized as integral representations of the Airy function Ai and its derivative Ai$'$. The change of variables is such that z_+ corresponds to $s_+ = \gamma$ and z_- to $s_- = -\gamma$. The reader is referred to [22] and/or [23] for a more complete discussion, including cautionary remarks about the proper choice of branch for the change of variables from z to s.

The formulas (C14)–(C20) and (6.15) provide the needed large k expansion that is uniformly valid in α. In order to present the results of working out these formulas for the integral (C12) in a compact form, make the definitions

$$v(\delta) = \frac{3}{8\delta^3}\left[\ln\left(\frac{1-\delta}{1+\delta}\right) + 2\delta + \frac{2}{3}\delta^3\right], \quad \text{(C21)}$$

$$u(\delta) = \left[\frac{(\alpha^4-1)\alpha^2}{4\lambda} - \frac{(\alpha^4+2)\alpha^2\delta^2}{16\lambda} - \frac{\alpha^6\delta^4}{16\lambda} + (2k+1)v(\delta)\right]^{1/3}, \quad \text{(C22)}$$

$$q_2 = (2q_0)^{1/2}, \quad \text{(C23)}$$

$$q_3 = (q_1 + q_2)^{1/2}, \quad \text{(C24)}$$

$$q_4 = \alpha^2 q_3^{-2}. \quad \text{(C25)}$$

The results, together with a few key intermediate steps, are

$$\gamma = \delta u(\delta), \quad \text{(C26)}$$

$$\rho = \frac{[\alpha^4(1+\delta^2) - 4]q_1}{24\lambda} + \frac{1}{4}(2k+1)\ln\left(\frac{q_1-\alpha^2}{q_1+\alpha^2}\right), \quad \text{(C27)}$$

$$\left[\mp\frac{1}{\delta}\left(\frac{d^2w}{dz^2}\right)_{z=z_\pm}\right]^{-1/2} = \frac{(\alpha^2 \pm q_1\delta)^{1/2}}{2^{1/2}\lambda^{1/4}q_1^{1/2}z_\pm^{1/2}}, \quad \text{(C28)}$$

$$g(z_\pm) = -2i\pi^{-1/2}\lambda^{1/4}C_+(\alpha^2 \pm q_1\delta)^{-1/2}B_2(z_\pm), \quad \text{(C29)}$$

$$z_\pm^{-1/2} = \lambda^{1/4}q_2^{-1}q_3(1 \mp q_4\delta), \quad \text{(C30)}$$

$$G_0(z_\pm) = -2i\pi^{-1/2}C_+q_1^{-1/2}[u(\delta)]^{1/2}z_\pm^{-1/2}B_2(z_\pm), \quad \text{(C31)}$$

$$a_0 = -2i\pi^{-1/2}C_+\lambda^{3/4}q_1^{-1/2}q_2^{-3}q_3^3[u(\delta)]^{1/2} \times[1 + 3q_4^2\delta^2 + b_1\lambda^{1/2}q_2^{-2}q_3^2(1 + 10q_4^2\delta^2 + 5q_4^4\delta^4) + b_2\lambda q_2^{-4}q_3^4(1 + 21q_4^2\delta^2 + 35q_4^4\delta^4 + 7q_4^6\delta^6)], \quad \text{(C32)}$$

$$a_1 = 2i\pi^{-1/2}C_+\alpha^2\lambda^{3/4}q_1^{-1/2}q_2^{-3}q_3[u(\delta)]^{-1/2} \times[3 + q_4^2\delta^2 + b_1\lambda^{1/2}q_2^{-2}q_3^2(5 + 10q_4^2\delta^2 + q_4^4\delta^4) + b_2\lambda q_2^{-4}q_3^4(7 + 35q_4^2\delta^2 + 21q_4^4\delta^4 + q_4^6\delta^6)]. \quad \text{(C33)}$$

The large k expansion that is uniformly valid in α is obtained by using (C26), (C27), (C32), and (C33) in (6.15). These formulas remain well behaved as the saddle points z_+ and z_- move from the real axis for $k < k_c$ (where δ is real) through coalescence at $k = k_c$ (where $\delta = 0$) out into the complex plane for $k > k_c$ (where δ is pure imaginary). When δ is small, the function $v(\delta)$ defined by (C21) should be evaluated from the power series

$$v(\delta) = -\frac{3}{4}\sum_{m=0}^{\infty}\frac{\delta^{2m+2}}{2m+5}. \qquad (C34)$$

When δ is pure imaginary and not small, the formula

$$v(iy) = \frac{3}{4y^3}\left[\tan^{-1}(y) - y + \tfrac{1}{3}y^3\right] \qquad (C35)$$

can be used.

[1] T. Kato, Commun. Pure Appl. Math. **10**, 151 (1957).
[2] C. Schwartz, Method Comput. Phys. **2**, 241 (1963).
[3] W. Lakin, J. Chem. Phys. **43**, 2954 (1965).
[4] B. Klahn and J. D. Morgan III, J. Chem. Phys. **81**, 410 (1984).
[5] R. N. Hill, J. Chem. Phys. **83**, 1173 (1985).
[6] J. D. Morgan III, in *Numerical Determination of the Electronic Structure of Atoms, Diatomic and Polyatomic Molecules*, Vol. 271 of *NATO Advanced Study Institute, Series C: Mathematical and Physical Sciences*, edited by Mireille Defranceschi and Joseph Delhalle (Kluwer, Dordrecht, 1989), pp. 49–84.
[7] W. Kutzelnigg and J. D. Morgan III, J. Chem. Phys. **96**, 4484 (1992).
[8] W. Klopper and W. Kutzelnigg, J. Mol. Struct. **135**, 339 (1986).
[9] W. Kutzelnigg, in *Strategies and Applications in Quantum Chemistry. A Tribute to G. Berthier*, edited by M. Defranceschi and Y. Ellinger (Kluwer, Dordrecht, 1994).
[10] W. Kutzelnigg, Int. J. Quantum Chem. **51**, 447 (1994).
[11] A. Erdelyi, W. Magnus, F. Oberhettinger, and F. G. Tricomi, *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), Vol. 2.
[12] W. Magnus, F. Oberhettinger, and R. P. Soni, *Formulas and Theorems for the Special Functions of Mathematical Physics*, 3rd ed. (Springer, New York, 1966).
[13] E. A. Hylleraas and B. Undheim, Z. Phys. **65**, 759 (1930).
[14] J. K. L. MacDonald, Phys. Rev. **43**, 830 (1933).
[15] Alexander Weinstein and William Stenger, *Methods of Intermediate Problems for Eigenvalues — Theory and Ramifications* (Academic, New York, 1972).
[16] *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1965).
[17] F. W. J. Olver, J. Res. Natl. Bur. Stand. Sect. B **63**, 131 (1959).
[18] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics—Non-relativistic Theory* (Pergamon, London, 1958).
[19] A. Erdelyi, W. Magnus, F. Oberhettinger, and F. G. Tricomi, *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), Vol. 1.
[20] R. N. Hill, J. Math. Phys. **21**, 2182 (1980).
[21] Philip M. Morse and Herman Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), Vol. 1.
[22] N. Bleistein and R. A. Handelsman, *Asymptotic Expansions of Integrals* (Holt, Rinehart, & Winston, New York, 1975).
[23] R. Wong, *Asymptotic Approximations of Integrals* (Academic, San Diego, 1989).
[24] F. W. J. Olver, *Asymptotics and Special Functions* (Academic, New York, 1974).
[25] R. E. Langer, Trans. Am. Math. Soc. **33**, 23 (1931); **34**, 447 (1932).
[26] S. C. Miller, Jr. and R. H. Good, Phys. Rev. **94**, 1345 (1954).
[27] G. Szegö, *Orthogonal Polynomials*, 4th ed. (American Mathematical Society, Providence, RI, 1975).
[28] A. Erdélyi and C. A. Swanson, *Asymptotic Forms of Whittaker's Confluent Hypergeometric Functions*, Memoirs of the American Mathematical Society No. 25 (American Mathematical Society, Providence, RI, 1957).
[29] H. Skovgarrd, *Uniform Asymptotic Expansions of Confluent Hypergeometric Functions and Whittaker Functions* (Gjellerups, Copenhagen, 1966).
[30] G. N. Watson, Proc. London Math. Soc. Ser. 2, **17**, 116 (1918).
[31] M. Wyman and R. Wong, Can. J. Math. **21**, 1013 (1969).
[32] E. W. Barnes, Philos. Trans. R. Soc. London Ser. A **206**, 249 (1906).
[33] Robert C. Forrey and Robert Nyden Hill, Ann. Phys. (N.Y.) **226**, 88 (1993).
[34] F. Stenger, SIAM Rev. **23**, 165 (1981).
[35] F. Stenger, *Numerical Methods Based on Sinc and Analytic Functions* (Springer, New York, 1993).
[36] J. Lund and K. L. Bowers, *Sinc Methods for Quadrature and Differential Equations* (SIAM, Philadelphia, 1992).
[37] R. E. Meyer, SIAM Rev. **31**, 435 (1989).