$1/R$ expansion for H_2^+: Calculation of exponentially small terms and asymptotics

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The energy of any bound state of the hydrogen molecule ion H_2^+ has an expansion in inverse powers of the internuclear distance R of the form

$$E(R)\sim \sum_N E^{(N)}(2R)^{-N}+e^{-R/n}\sum_N A^{(N)}(2R)^{-N} + e^{-2R/n}\left[\sum_N B^{(N)}(2R)^{-N}+\ln(R)\text{ terms}\right] \pm ie^{-2R/n}\sum_N C^{(N)}(2R)^{-N}+\cdots .$$

Rayleigh-Schrödinger perturbation theory (RSPT) gives the coefficients $E^{(N)}$ but is otherwise unable to treat the exponentially small series, which in part are characteristic of the double-well aspect of H_2^+. (Here n denotes the hydrogenic principal quantum number.) We develop a quasisemiclassical method for solving the Schrödinger equation that gives all the exponentially small subseries. The RSPT series diverges: for the ground state $E^{(N)}\sim -(N+1)!/e^2$ for large N. The $E^{(N)}$ asymptotics are governed via a dispersion relation by the imaginary $e^{-2R/n}$ series, which itself is given by the square of the $e^{-R/n}$ series times a "normalization integral." That the expansion itself contains imaginary terms might seem inconsistent with the reality of the H_2^+ eigenvalues. In fact, the RSPT series is Borel summable for R complex. The Borel sum has a cut on the real R axis, and its limit from above or below the positive R axis is complex. The imaginary $e^{-2R/n}$ (and higher) series consist of just the counterterms to cancel the imaginary part of the Borel sum. Extensive numerical examples are given. Of interest is a weak (down by a factor N^{-6}) alternating-sign contribution to $E^{(N)}$, which is uncovered both theoretically and numerically. Also of interest is the identification of the Borel sum of the RSPT series with nonphysical boundary conditions. This too is illustrated both theoretically and numerically.

I. INTRODUCTION

This paper is about the expansion of the energy of the hydrogen molecule ion H_2^+ in powers of $(2R)^{-1}$, R being the internuclear distance. Of course, H_2^+ has special importance as a prototype for molecular binding and for double wells, but it is generally regarded as simple, well understood,[1–4] and perhaps not very interesting. Exactly the opposite is true: the study of H_2^+ at large R has revealed several unexpected features.[5,6]

We list in this introduction seven main results. The first is that (i) the energy of any bound state is given formally by an explicitly computable *complex* expansion that is *discontinuous* across the positive R axis,

$$E(R)\sim \sum_N E^{(N)}(2R)^{-N}+e^{-R/n}\sum_N A^{(N)}(2R)^{-N} +e^{-2R/n}\left[\sum_N B^{(N)}(2R)^{-N}+\ln(R)\text{ terms}\right] \pm ie^{-2R/n}\sum_N C^{(N)}(2R)^{-N}+\cdots \quad (1)$$

Here the $\pm$ is the sign of ImR, and n is the hydrogenic principal quantum number. When R is real, then the sign indicates whether it has become real from above or below the real axis.

More surprising is that (ii) the "sum" of the explicitly complex series (1) is both real and continuous across the positive R axis. The explicit imaginary series is canceled by an implicit imaginary contribution from the sum of the ordinary, real, divergent Rayleigh-Schrödinger perturbation-theory (RSPT) expansion, $\sum_N E^{(N)}(2R)^{-N}$. This remarkable subtlety involves taking the sum of the divergent RSPT series to be the analytic continuation back to the real axis of the Borel sum, which exists for R complex;[6] this is equivalent, as we shall see,[7] to recognizing that $R>0$ is a Stokes line of the expansion. (A similar cancellation in part has been noticed by Zinn-Justin for the double-well oscillator.[8–10])

This paper is also about the method used to generate the solution of the eigenvalue problem by asymptotic expansion—the quasisemiclassical (QSC) method. Through the separability of the H_2^+ eigenvalue equation in prolate spheroidal coordinates,[11] which here involves two separation constants β_1 and β_2, a systematic procedure is developed to generate the RSPT series, the $e^{-R/n}$ double-well gap series, the $e^{-2R/n}$ real and imaginary series, and so forth. Of course ordinary RSPT gets only the first of these series.

The third specific result concerns the relationship between the imaginary $ie^{-2R/n}$ series and the $e^{-R/n}$ "gap" series. These two series arise primarily from the separation constant β_2 for which (iii) the corresponding imaginary series as πi times the square of the corresponding gap series times a normalization constant.

Other main points include the following. (iv) The H_2^+ eigenvalue equation has complex eigenvalues closely associated with the real eigenvalues in the sense that they have the same RSPT, but involve different boundary conditions.[5,6] The "different boundary conditions" can be understood in a simple way by considering the analytic continuation of one of the separated equations of a related, physically interpretable problem:[5,6] an electron moving in the field of a fixed proton and a fixed antiproton. (v) RSPT for β_2 is Borel summable to the complex eigenvalues.[5,6] (vi) The imaginary series determine the large-order behavior of the RSPT coefficients via dispersion relations. (vii) The imaginary series associated with the discontinuity of the separation constant β_1 across the negative real axis has logarithmic terms in $-R$, which lead to $\ln(N)$ terms in the asymptotics of the $\beta_1^{(N)}$ and $E^{(N)}$.

Two empirical facts have been our main motivation. The first is the same-sign factorial divergence of the RSPT series for the ground state:[3,12–14]

$$E^{(N)}\sim -(N+1)!e^{-2}\left[1+\frac{2}{N+1}-\frac{18}{(N+1)N}+\cdots\right]. \quad (2)$$

Such behavior is consistent with the asymptotic expansion of a *complex* function that is discontinuous across the $R>0$ axis, whose Borel sum would be like

$$-\sum_{N=0}^{\infty}(N+1)!e^{-2}(2R)^{-N}\sim e^{-2}\int_0^\infty t^2e^{-t}(t-2R)^{-1}dt \quad [0<|\arg(R)|<2\pi] \quad (3)$$

$$=\mathrm{P}e^{-2}\int_0^\infty t^2e^{-t}(t-2R)^{-1}dt\pm i\pi 4R^2e^{-2R-2}\quad (\mathrm{Im}R=\pm 0)\,. \quad (4)$$

where P denotes the principal value of the integral. The second empirical fact is an approximate relationship[12] between the double-well energy gap E_{gap}, which for the pair consisting of the ground and first excited state is $\sim 4Re^{-R-1}$, and the asymptotics of the RSPT coefficients [Eq. (2)], which by a dispersion relation involves the "$\pm$" discontinuity in Eq. (1). The relationship is

$$\text{discontinuity in Eq. (1)} \sim 2\pi i(\tfrac{1}{2}E_{\text{gap}})^2\,. \quad (5)$$

Our initial goal was to explain both facts, but in the process we have obtained many more results, which have been summarized in Ref. 5. Further, in Ref. 6, the first of two papers announced in Ref. 5, we have collected the mathematically rigorous results: proof of the analyticity of β_1, β_2, and E; proof of Borel summability of the RSPT series for β_1, β_2, and E to eigenvalues of non-self-adjoint versions of the H_2^+ problem; proof of the approximate formula (5); justification of the dispersion relations; and justification of the leading asymptotic behavior of the RSPT coefficients. This paper is the second paper announced in Ref. 5 in which we develop the QSC technique, derive the multiply-exponentially-small series, and obtain the full high-order asymptotics of the RSPT quantities, i.e., all the corrections in formula (2) for the ground state and for excited states as well.

The organization of the paper is briefly as follows. In Sec. II, the Schrödinger equation is separated, and the RSPT solution is sketched. Section III is a long section devoted to the separation constant β_2, which comes from the separated equation that contains the double-well character of H_2^+. In Sec. III A, the quasisemiclassical method is introduced through the form of the wave function, and the separated Schrödinger equation is turned into a Riccati equation. In Sec. III B, the recursive, perturbative solution of the Riccati equation is sketched, and the usual

RSPT is shown to fall out. In Sec. III C, it is shown how the second boundary condition, ignored by RSPT for H_2^+, leads to the double-well gap and to exponentially small (e^{-R}) terms. Sections III D and III E give alternative formulas for quantities that appear first in Sec. III C. How *imaginary* terms occur in the expansion for β_2 is first introduced in Sec. III F and further developed in Sec. III G, where the "gap-squared" formula is discussed. The doubly-exponentially-small series contributing to β_2 is obtained in Sec. III H. The final subsection, III I, is a mathematical diversion from the physical H_2^+ problem: the β_2 equation is solved not on the finite physical interval, but on a semiinfinite interval. As mentioned in (v) above, the resulting eigenvalue turns out to be the Borel sum of the RSPT series, and the series for the discontinuity in the Borel sum across its cut is given by the imaginary series obtained in Sec. III G. Section IV contains the details for the solution of the separation constant β_1. In Sec. V the two separation constants are put back together to get the energy $E(R)$. The details are mostly algebraic, but nontrivial. In Sec. V C the (appropriate) approximate, gap-squared formula of Brézin and Zinn-Justin is shown to be true for exactly two terms for all states, not just the ground state. In Sec. V E the discontinuity in $E(R)$ for R negative is discussed in preparation for the development of the asymptotics of the RSPT coefficients via dispersion relations in Sec. VI. Section VII contains a JWKB-like reformulation of the method that is easier to use for numerical calculations of the various series, which calculations are discussed and illustrated in Secs. VIII—X. Summation of the expansions and comparison with direct numerical solution of the eigenvalue equations are discussed in Sec. XI. All of the quantities discussed are illustrated numerically in extensive tables, and the paper is summarized in Sec. XII.

II. PRELIMINARIES: SEPARATION OF VARIABLES; RSPT RESULTS

The aims of this preliminary section are to give the separated equations for H_2^+ in prolate spheroidal coordinates,[11] to indicate how to carry out RSPT on them, to state the asymptotic RSPT results, and to set out the notation. The RSPT results serve both as part of the motivation and as a point of departure for the QSC treatment that follows in Sec. III. (For the implementation of the separability in terms of operator theory in Hilbert space, see Ref. 6.)

A. Separated equations in prolate spheroidal coordinates

Prolate spheroidal coordinates, with a translation to make the left endpoints for the ξ and η both be 0, are given by[11]

$$\xi \equiv (r_a+r_b)/R-1 \quad (0\le\xi<\infty)\ , \tag{6}$$

$$\eta \equiv (r_a-r_b)/R+1 \quad (0\le\eta\le 2)\ , \tag{7}$$

$$\phi \equiv \arctan(y/x)\ . \tag{8}$$

The dependence of the wave function on ϕ is the familiar and simple $e^{im\phi}$ (m an integer). The dependence on ξ and η is what needs to be determined.

The Schrödinger equation,

$$H\Psi=(-\tfrac{1}{2}\nabla^2-1/r_a-1/r_b+1/R)\Psi=(E+1/R)\Psi\ , \tag{9}$$

yields two equations for the separation constants β_1 and β_2,

$$\left[-\frac{d^2}{d\xi^2}+\frac{1}{4}r^2-r\frac{\beta_1}{\xi}-r\frac{\beta_1+2\beta_2}{\xi+2}+\frac{m^2-1}{\xi^2(\xi+2)^2}\right]\Phi_1=0\ , \tag{10}$$

$$\left[-\frac{d^2}{d\eta^2}+\frac{1}{4}r^2-r\frac{\beta_2}{\eta}-r\frac{\beta_2}{2-\eta}+\frac{m^2-1}{\eta^2(2-\eta)^2}\right]\Phi_2=0\ , \tag{11}$$

with the energy E being obtained from β_1 and β_2 by the formula

$$E=-\tfrac{1}{2}(\beta_1+\beta_2)^{-2}\ . \tag{12}$$

Equation (12) and the familiar expression for the hydrogen-atom energy eigenvalue, $-\frac{1}{2}n^{-2}$, show that $\beta_1+\beta_2$ may be regarded as a "perturbed principal quantum number n." The r in Eqs. (10) and (11) is a scaled version of the internuclear distance R:

$$r\equiv R/(\beta_1+\beta_2)\sim R/n\ . \tag{13}$$

B. Manipulation of the separated equations into standard RSPT form

Despite the nonstandard form of Eqs. (10)—(13), it is straightforward to develop solutions by RSPT. We begin with a scale transformation that makes the unperturbed problem hydrogenic:

$$u=r\xi,\quad v=r\eta\ , \tag{14}$$

$$[-u\,d^2/du^2+\tfrac{1}{4}u+\tfrac{1}{4}(m^2-1)/u]\Phi_1+uV_1(u,\beta_1+2\beta_2,r)\Phi_1=\beta_1\Phi_1\ , \tag{15}$$

$$[-v\,d^2/dv^2+\tfrac{1}{4}v+\tfrac{1}{4}(m^2-1)/v]\Phi_2+vV_2(v,\beta_2,r)\Phi_2=\beta_2\Phi_2\ . \tag{16}$$

The expression that occurs in square brackets in Eqs. (15) and (16) is identical with the separated "Hamiltonians" for the hydrogen atom in parabolic coordinates:[15,16] we take it as the unperturbed Hamiltonian for both problems. Notice also that the factors u and v in $u\,d^2/du^2$ and $v\,d^2/dv^2$ imply that the volume elements are $u^{-1}du$ and $v^{-1}dv$. Thus the unperturbed eigenfunctions are identical with the parabolic hydrogenic eigenfunctions, and the unperturbed separation constants are

$$\beta_i=\beta_i^{(0)}=n_i+\tfrac{1}{2}(|m|+1)\quad(i=1,2,\ r=+\infty)\ , \tag{17}$$

where n_1 and n_2 are the usual parabolic quantum numbers.

We continue by expanding the perturbing potentials V_i in power series in $(2r)^{-1}$ (the perturbation expansions for the $\beta_i^{(N)}$ are defined below):

$$V_1(u,\beta_1+2\beta_2,r)=-\frac{\beta_1+2\beta_2}{u+2r}+\tfrac{1}{4}(m^2-1)\times\left[-\frac{2}{u(u+2r)}+\frac{1}{(u+2r)^2}\right] \quad (18)$$

$$=\sum_{N=1}^{\infty}V_1^{(N)}(2r)^{-N}, \quad (19)$$

$$V_1^{(N)}=\tfrac{1}{4}(m^2-1)(N+1)(-u)^{N-2}-\sum_{k=0}^{N-1}(\beta_1^{(k)}+2\beta_2^{(k)})(-u)^{N-k-1}, \quad (20)$$

$$V_2(v,\beta_2,r)=-\frac{\beta_2}{2r-v}+\tfrac{1}{4}(m^2-1)\left[\frac{2}{v(2r-v)}+\frac{1}{(2r-v)^2}\right] \quad (21)$$

$$=\sum_{N=1}^{\infty}V_2^{(N)}(2r)^{-N}, \quad (22)$$

$$V_2^{(N)}=\tfrac{1}{4}(m^2-1)(N+1)v^{N-2}-\sum_{k=0}^{N-1}\beta_2^{(k)}v^{N-k-1}. \quad (23)$$

Given the expansions (18)–(23), it is straightforward to solve Eqs. (15) and (16) by textbook RSPT. The first step is to obtain β_2 as a power series in $(2r)^{-1}$ by solving Eq. (16). The second step is to obtain the series for β_1 from Eq. (15) and the β_2 series. The third step is to obtain r^{-1} as a series in R^{-1} from Eq. (13), which then permits E to be expressed as a series in R^{-1}, the fourth and final step. Note that Eqs. (20) and (23) are strictly valid only when u and v are both less than $2r$. However, the RSPT solution is an asymptotic power series in $1/2r$, and the order-by-order equations, which are obtained for large $2r$, of course hold formally for all values of u and v. To look at it another way, if a nonperturbative solution were to be obtained, then by ignoring the corresponding expansions for u and v greater than $2r$, an error that is exponentially small in r would be introduced into the solution, which would again therefore be of no consequence for the $1/2r$ RSPT.

Note that β_1 and β_2 depend on m only through the magnitude $|m|$ and not on the sign. To simplify the appearance of the formulas, we assume from now on, *without loss of generality*, that $m\geq 0$.

C. RSPT results for the separation constants

The RSPT series for the separation constants have been calculated as outlined above. We shall not go into the relatively uninteresting details. At low order the series appear unremarkable. One finds for the ground state ($n_1=n_2=m=0$), for example, that

$$\beta_1\sim\sum_{N=0}^{\infty}\beta_1^{(N)}(2r)^{-N} \quad (24)$$

$$=0.5-(2r)^{-1}+3(2r)^{-2}+4(2r)^{-3}-15(2r)^{-4}+\cdots, \quad (25)$$

$$\beta_2\sim\sum_{N=0}^{\infty}\beta_2^{(N)}(2r)^{-N} \quad (26)$$

$$=0.5-(2r)^{-1}-(2r)^{-2}-4(2r)^{-3}-23(2r)^{-4}+\cdots. \quad (27)$$

What is especially significant is that at high order the $\beta_i^{(N)}$ for the ground state behave asymptotically as

$$\beta_2\sim-(N+1)!\left[1-\frac{6}{N+1}+\frac{2}{(N+1)N}-\frac{16}{(N+1)N(N-1)}-\cdots\right], \quad (28)$$

$$\beta_1\sim 2N!\left[1-\frac{6}{N}-\frac{8}{N(N-1)}+\frac{48}{N(N-1)(N-2)}+\cdots\right]. \quad (29)$$

The same-sign factorial divergence of the separation-constant coefficients, Eqs. (28) and (29), is the same phenomenon as the factorial divergence[3,13] of $E^{(N)}$, Eq. (2), discovered by Morgan and Simon.[3] This phenomenon is a main motivating fact for this study. In explaining the detailed relationships among the RSPT quantities and the exponentially small quantities associated with the double-well phenomena, we shall focus on the separation constants. It is easier to deal with the separation constants than with E directly, because the separation constants are eigenvalues of ordinary differential equations.

We conclude this section with a remark about the endpoints of the β_2 equation (16), which have been treated rather unequally in RSPT. By this we mean that since the unperturbed problem is defined on the semi-infinite interval, the influence of the second boundary condition is not seen by the perturbation theory. As a consequence typical of double-well problems, the characteristic splitting does not show up: both the symmetric and antisymmetric partners of a double-well pair have the same $1/2r$ RSPT expansion. The quasisemiclassical method developed in the next section deals explicitly with both boundary points and consequently gets the double-well splitting.

III. SOLUTION OF THE β_2 EQUATION BY THE QUASISEMICLASSICAL METHOD

Rayleigh-Schrödinger perturbation theory is unable to calculate the double-well gap. In this section we develop a method for solving the β_2 equation (11) that gives not only the gap, but also smaller more subtle effects, while still yielding within the same formalism the RSPT expansion. The *exact* relationship between the RSPT asymptotics and the square of the gap is found. The final formula we are led to for β_2 is a complex expansion whose explicit imaginary terms for real r are discontinuous across the positive axis. The explanation of this apparently paradoxical representation of a real, continuous function is that the Borel sum of the real RSPT expansion exists and has a cut on the positive r axis,[6] so that the value of the Borel sum continued to the real axis is complex, and the explicitly imaginary terms in the expansion are the counterterms that cancel the imaginary part of the Borel sum. This behavior turns out to be widespread: for examples in familiar functions, such as the Airy Bi function, see Ref. 7.

The Borel sum of the RSPT expansion for β_2 turns out[5,6] not to be the eigenvalue associated with Eq. (16), but to be the eigenvalue of a related problem. Consider Eq. (16) both at $-r$ and with a semi-infinite domain. That is, set $r'=-r$ in V_2 of Eq. (21):

$$V_2(v,\beta_2(-r'),-r')=\frac{\beta_2}{2r'+v}+\tfrac{1}{4}(m^2-1)\times\left[-\frac{2}{v(2r'+v)}+\frac{1}{(2r'+v)^2}\right]. \tag{30}$$

On the semi-infinite interval, $0\le v<\infty$, Eq. (16), with V_2 given by Eq. (30), represents a stable, single-well eigenvalue problem whose RSPT expansion is Borel summable[5,6] to the eigenvalue of that problem. That RSPT expansion is the same as for $\beta_2(r)$ with r replaced by $-r'$. This modified problem [Eq. (16) where V is defined by Eq. (30) on $0\le v<\infty$] arises naturally from the separation of the Schrödinger equation for an electron moving in the field of a proton and an antiproton.[5,6]

To bring out the connection of the Borel sum with the imaginary series for β_2 mentioned in the first paragraph of this section, we also solve here by the QSC method the β_2 eigenvalue problem on the semi-infinite interval $0\le v<\infty$, but without changing the sign of r. To avoid the singularity that would occur at $v=2r$, we make r complex. Then the QSC method yields an expansion for the discontinuity in the Borel sum at the $r>0$ axis that is exactly -2 times the imaginary series that occurs in the finite, $0\le v\le 2r$ β_2 problem, thus clinching the cancellation. (To leading exponential order only, the calculation of the discontinuity has been made completely rigorous. See Sec. IV of Ref. 6.)

The *method* we develop here is semiclassical. It is closest to the methods of Langer[17] and Cherry.[18] It differs from standard semiclassical practice in that a *singular point* of the differential equation, rather than a *classical turning point,* is the "anchor point" for the expansion, and exponentially small, subdominant terms can enter the actionlike function. To emphasize the similarities and differences, and for lack of a better term, we refer to the approach as the quasisemiclassical (QSC) method.

The basic idea of the QSC method is to make the perturbation expansion on the "natural variable" on which depends a function that represents the solution of the differential equation near one boundary or singular point. One converts the linear Schrödinger equation into a nonlinear, fourth-order Riccati equation for the natural variable that is solved perturbatively. To satisfy one boundary condition perturbatively, β_2 must be represented by its RSPT series. To satisfy both boundary conditions, β_2 must have an additional, exponentially small (e^{-r}) series that represents half the double-well gap between the symmetric and antisymmetric states of an associated pair. In fact there are additional series that are $O(e^{-2r})$, $O(e^{-3r})$, etc., that are found by satisfying both boundary conditions to higher exponentially small orders. (We stop at the e^{-2r} series.)

A. The quasisemiclassical wave function

The most direct way to characterize the QSC method is through the form of the wave function. The characteristic of the semiclassical Jeffreys-Wentzel-Kramers-Brillouin (JWKB) method[1] is that the logarithm of the wave function is expanded in a power series in $\hbar$. More precisely, the wave function is put in the form

$$\Psi_{\mathrm{JWKB}}=(dS/dx)^{-1/2}e^{iS/\hbar}, \tag{31}$$

$$S=\sum_{N=0}^{\infty}S^{(N)}(x)\hbar^{2N}, \tag{32}$$

where $S^{(0)}$ is the classical action, and where the corrections $S^{(N)}$ ($N\ge 1$) are determined recursively.

The JWKB method fails at the classical turning points, where the $S^{(N)}(x)$ may have singularities. Langer[17] generalized the JWKB method to include the classical turning points in part by solving the differential equation itself at the turning point in terms of Airy functions. Away from a turning point the Airy functions can be expanded asymptotically, and Langer's method goes over into the JWKB method.

The points of special interest in the β_2 equation (11) are $\eta=0$ and 2—which are singular points rather than turning points. (The JWKB method fails even more strongly at singularities.) Near $\eta=0$, Eq. (11) is

$$\left[-\frac{d^2}{d\eta^2}+\frac{1}{4}r^2-r\frac{\beta_2}{\eta}+\frac{m^2-1}{4\eta^2}\right]\Phi_2\sim 0, \tag{33}$$

which up to rescaling is Whittaker's confluent hypergeometric equation, whose solution[19,20] regular at 0 is denoted by $M_{\beta_2,m/2}(r\eta)$. In the spirit of Langer's generalization, we take the solution of Eq. (11) near $\eta=0$ to have the form

$$\Phi_2=\frac{1}{m!}(d\phi/d\eta)^{-1/2}M_{b,m/2}(r\phi). \tag{34}$$

The Whittaker M function here plays the role of the Airy function in Langer's method, while $1/r$ is like $\hbar$. The value of the index b will be clarified later. The problem of determining the solution Φ_2 of Eq. (11) then becomes the problem of determining the function $\phi=\phi(\eta,r)$, which by Eqs. (11), (33), and (34) satisfies the Riccati equation

$$-\left[\frac{d\phi}{d\eta}\right]^2\left[\frac{1}{4}-\frac{b}{r\phi}+\frac{m^2-1}{4r^2\phi^2}\right]-\frac{1}{r^2}\left[\frac{d\phi}{d\eta}\right]^{1/2}\frac{d^2}{d\eta^2}\left[\frac{d\phi}{d\eta}\right]^{-1/2}+\frac{1}{4}-\frac{\beta_2}{r}\left[\frac{1}{\eta}+\frac{1}{2-\eta}\right]+\frac{m^2-1}{4r^2}\left[\frac{1}{\eta}+\frac{1}{2-\eta}\right]^2=0\,. \tag{35}$$

Cherry[18] extended Langer's approach by expanding the function corresponding here to ϕ as a power series in a parameter that here is $(2r)^{-1}$:

$$\phi(\eta,r)\sim\sum_{N=0}^{\infty}\phi^{(N)}(\eta)(2r)^{-N}\,. \tag{36}$$

Thus the problem of determining Φ_2 becomes the problem of determining the $\phi^{(N)}$.

The parameter b in the Whittaker function is ultimately determined by making Φ_2 satisfy both boundary conditions. We anticipate that it is equal to the unperturbed value of β_2 to zeroth exponential order:

$$b=\beta_2^{(0)}+O(r^ke^{-r})\quad(\text{for some }k>0)\,. \tag{37}$$

Then $M_{\beta_2^{(0)},m/2}(r\eta)$ is simply the usual RSPT unperturbed wave function,[1,16] i.e., a polynomial in η times $\eta^{m/2+1/2}e^{-r\eta/2}$. This value of b turns out to simplify both the analytic form of the $\phi^{(N)}$ and also the asymptotic analysis of $M_{b,m/2}$ that is needed to match the boundary condition at $\eta=2$. (Later it will also be necessary to add exponentially small terms to b, to ϕ, and to β_2 when the process of satisfying both boundary conditions is extended to higher exponential order.)

B. Equations satisfied by the $\phi^{(N)}$; explicit solution for $\phi^{(0)}$, $\phi^{(1)}$, and $\phi^{(2)}$; RSPT for $\beta_2^{(1)}$

To provide a concrete example and to illustrate how RSPT "falls out," we calculate $\phi^{(0)}$, $\phi^{(1)}$, $\phi^{(2)}$, and $\beta_2^{(1)}$ explicitly.

Put the expansions (36) for ϕ, (26) for β_2, and (37) for b into the Riccati equation (35), which can then be solved recursively. To lowest order in $(2r)^{-1}$, one finds

$$-\tfrac{1}{4}(d\phi^{(0)}/d\eta)^2+\tfrac{1}{4}=0\,, \tag{38}$$

$$d\phi^{(0)}/d\eta=1,\quad \phi^{(0)}=\eta\,. \tag{39}$$

Note that the unperturbed value of ϕ is η, consistent with the discussion above [between Eqs. (33) and (34)] of Φ_2 near $\eta=0$. Moreover, since Φ_2 at $\eta=0$ behaves like

$$\Phi_2\sim\eta^{m/2+1/2}\,, \tag{40}$$

the equivalent condition for ϕ is

$$\phi^{(N)}=O(\eta)\quad\text{as }\eta\to 0\,, \tag{41}$$

which also explains the choice of "integration constant" in Eq. (39).

To first order in $(2r)^{-1}$, Eqs. (35)–(41) yield

$$-\frac{1}{2}\frac{d\phi^{(1)}}{d\eta}+2\beta_2^{(0)}\frac{1}{\eta}-2\beta_2^{(0)}\left[\frac{1}{\eta}+\frac{1}{2-\eta}\right]=0\,, \tag{42}$$

$$\phi^{(1)}=4\beta_2^{(0)}\ln(1-\tfrac{1}{2}\eta)\,. \tag{43}$$

To second order in $(2r)^{-1}$, Eqs. (35)–(43) yield

$$-\frac{1}{2}\frac{d\phi^{(2)}}{d\eta}-\frac{1}{4}\left[\frac{d\phi^{(1)}}{d\eta}\right]^2+4\beta_2^{(0)}\frac{1}{\phi^{(0)}}\frac{d\phi^{(1)}}{d\eta}-2\beta_2^{(0)}\frac{\phi^{(1)}}{(\phi^{(0)})^2}-(m^2-1)\frac{1}{(\phi^{(0)})^2}-2\beta_2^{(1)}\left[\frac{1}{\eta}+\frac{1}{2-\eta}\right]+(m^2-1)\left[\frac{1}{\eta}+\frac{1}{2-\eta}\right]^2=0\,, \tag{44}$$

$$d\phi^{(2)}/d\eta=-16(\beta_2^{(0)})^2\eta^{-2}\ln(1-\tfrac{1}{2}\eta)-16(\beta_2^{(0)})^2\eta^{-1}(2-\eta)^{-1}+2[-4(\beta_2^{(0)})^2+m^2-1]\frac{1}{(2-\eta)^2}+2[-2\beta_2^{(1)}+m^2-1-4(\beta_2^{(0)})^2]\left[\frac{1}{\eta}+\frac{1}{2-\eta}\right]\,, \tag{45}$$

$$\phi^{(2)}=16(\beta_2^{(0)})^2[\eta^{-1}\ln(1-\tfrac{1}{2}\eta)+\tfrac{1}{2}]+2[-4(\beta_2^{(0)})^2+m^2-1][(2-\eta)^{-1}-\tfrac{1}{2}]+2[-2\beta_2^{(1)}+m^2-1-4(\beta_2^{(0)})^2]\ln[\eta/(2-\eta)]\,. \tag{46}$$

Equation (46) would display a singularity in $\phi^{(2)}$ at $\eta=0$ *unless*

$$\beta_2^{(1)}=-2(\beta_2^{(0)})^2+\tfrac{1}{2}(m^2-1)\,, \tag{47}$$

which is precisely the RSPT result. Then instead of Eq. (46), $\phi^{(2)}$ is given by

$$\phi^{(2)}=16(\beta_2^{(0)})^2[\eta^{-1}\ln(1-\tfrac{1}{2}\eta)+\tfrac{1}{2}]+4\beta_2^{(1)}[(2-\eta)^{-1}-\tfrac{1}{2}]\,. \tag{48}$$

The equations for $\phi^{(3)},\phi^{(4)},\ldots$ get progressively more tedious. However, each $\phi^{(N)}$ can be found in closed form; each $\phi^{(N)}$ is analytic and has a zero at $\eta=0$, provided only that $\beta_2^{(N-1)}$ is chosen correctly. In fact it is not hard to show inductively from Eqs. (35), (39), (43), and (48) that $\beta_2^{(N-1)}$ can be chosen to make $\phi^{(N)}$ analytic and zero at $\eta=0$. By the uniqueness of power series, the $\beta_2^{(N)}$—determined so that the QSC Φ_2 satisfy the boundary condition at $\eta=0$—must be identical with the RSPT $\beta_2^{(N)}$. In this way the QSC method contains RSPT.

C. Boundary condition at $\eta=2$ and the double-well gap

A major advantage of the QSC method over RSPT is that the wave function can be made to vanish at $\eta=2$, as will now be demonstrated. The basic idea is to generate QSC wave functions from both $\eta=0$ and 2 and to match them in the middle where the asymptotic expansion for the Whittaker function is valid. A most crucial detail, however, is that the exponentially small shift [Eq. (37)] in the b index of the Whittaker function of Eq. (34) must now be determined. To find this shift, we reexamine the perturbation hypothesis—namely, that β_2 and ϕ can be expanded in power series in $(2r)^{-1}$.

As is well known, the RSPT expansion for β_2 is incomplete in the sense that there is an exponentially small correction of the form[2,4]

$$\beta_2 \sim \sum_{N=0}^{\infty} \beta_2^{(N)}(2r)^{-N} + \Delta\beta_2^{\{1\}} + O(r^k e^{-2r}) \quad (\text{for some } k>0)\,, \tag{49}$$

$$\Delta\beta_2^{\{1\}} \sim \pm\frac{(2r)^{2\beta_2^{(0)}} e^{-r}}{n_2!(n_2+m)!}\,. \tag{50}$$

The notation $\Delta f^{\{q\}}$ is to signify that part of f that is proportional to e^{-qr}. The quantity $2\Delta\beta_2^{\{1\}}$ is the double-well splitting [through $O(e^{-r})$] that separates the symmetric and antisymmetric states of a double-well pair, both of which have the same RSPT expansion. To make it possible to calculate the exponentially small terms, it is necessary to add them to the perturbation expansions (24) and (26) for β_1 and β_2, and to permit them to enter the expansions (37) for b and (36) for ϕ. This generalization is a natural but marked departure from the usual semiclassical practice. We put

$$\beta_i \sim \sum_{N=0}^{\infty} \beta_i^{(N)}(2r)^{-N} + \Delta\beta_i^{\{1\}} + O(r^k e^{-2r}) \quad (i=1,2)\,, \tag{51}$$

$$b \sim \beta_2^{(0)} + \Delta b^{\{1\}} + O(r^k e^{-2r})\,, \tag{52}$$

$$\phi(\eta,r) \sim \sum_{N=0}^{\infty} \phi^{(N)}(\eta)(2r)^{-N} + \Delta\phi^{\{1\}} + O(r^k e^{-2r})\,. \tag{53}$$

[In Eqs. (51)—(53) and in all subsequent equations, we omit the generic "for some $k>0$," which without danger of confusion may be taken as understood.] It will be seen later that the leading terms of $\Delta\beta_2^{\{1\}}$ and $\Delta b^{\{1\}}$ are equal:

$$\Delta\beta_2^{\{1\}} = \Delta b^{\{1\}}[1+O(r^{-1})] = \pm\frac{(2r)^{2\beta_2^{(0)}} e^{-r}}{n_2!(n_2+m)!}[1+O(r^{-1})]\,. \tag{54}$$

The crucial role played by the shift in the b index is immediately apparent when, in preparation for matching the wave function (34) with one satisfying the boundary condition at $\eta=2$, the Whittaker M function is expanded asymptotically:[20]

$$\frac{1}{m!}M_{b,m/2}(z) = \frac{e^{\pm\pi i(m/2+1/2-b)}}{\Gamma(\frac{1}{2}m+\frac{1}{2}+b)}W_{b,m/2}(z) + \frac{e^{\mp\pi i b}}{\Gamma(\frac{1}{2}m+\frac{1}{2}-b)}W_{-b,m/2}(ze^{\mp\pi i}) \quad (0<\pm\arg z<\pi) \tag{55}$$

$$\sim \frac{e^{\pm\pi i(m/2+1/2-b)}}{\Gamma(\frac{1}{2}m+\frac{1}{2}+b)} z^b e^{-z/2}\,{}_2F_0(\tfrac{1}{2}+\tfrac{1}{2}m-b, \tfrac{1}{2}-\tfrac{1}{2}m-b;;-z^{-1}) + \frac{1}{\Gamma(\frac{1}{2}+\frac{1}{2}m-b)} z^{-b}e^{+z/2}\,{}_2F_0(\tfrac{1}{2}+\tfrac{1}{2}m+b, \tfrac{1}{2}-\tfrac{1}{2}m+b;;+z^{-1}) \quad (0<\pm\arg z<\pi) \tag{56}$$

$$\sim (-1)^{n_2}\frac{e^{\mp\pi i\Delta b^{\{1\}}}}{(n_2+m)!} z^b e^{-z/2} + \Delta b^{\{1\}}(-1)^{n_2+1} n_2!\, z^{-b} e^{+z/2} \quad (0<\pm\arg z<\pi)\,, \tag{57}$$

where we have used the Γ-function reflection formula[19] and that $b+\frac{1}{2}-\frac{1}{2}m \sim n_2+1+\Delta b^{\{1\}}$ to get

$$1/\Gamma(\tfrac{1}{2}+\tfrac{1}{2}m-b) = \Gamma(b+\tfrac{1}{2}-\tfrac{1}{2}m)\pi^{-1}\sin[\pi(b+\tfrac{1}{2}-\tfrac{1}{2}m)] \tag{58}$$

$$= (-1)^{n_2+1} n_2!\,\Delta b^{\{1\}}[1+O(\Delta b^{\{1\}})]\,. \tag{59}$$

Note the introduction in Eq. (55) of the Whittaker W functions, primarily for later use, and in Eq. (56) the usual generalized hypergeometric series,[19]

$${}_2F_0(a,b;;z) = 1 + ab\frac{z}{1!} + a(a+1)b(b+1)\frac{z^2}{2!} + \cdots\,. \tag{60}$$

When $\Delta b^{\{1\}} \neq 0$, there is a *positive exponential term* in Φ_2. Consider for the moment how Φ_2 appears near the point $\eta=2$. The positive exponential in Eqs. (56) and (57) (where $z=r\phi \sim r\eta$) is the term that is *decaying* away from $\eta=2$ (in the direction of $\eta=0$) and near $\eta=2$ should be the most important term. In fact, because of the symmetry of Eq. (11), Φ_2 should be either symmetric or antisymmetric under the transformation $\eta \to 2-\eta$, so that both exponentials should be equally weighted. It will turn out that $\Delta b^{\{1\}}$ has exactly the right value to achieve this symmetry.

It is now straightforward to obtain the leading terms in the asymptotic expansion of Φ_2. Take $\phi^{(0)}$ and $\phi^{(1)}$ from Eqs. (39) and (43), and use Eqs. (34) and (57) to obtain, for Φ_2 anchored at $\eta=0$ (denoted here by $\Phi_{2[0]}$),

$$\Phi_{2[0]} \sim \frac{(-1)^{n_2}(2r)^{\beta_2^{(0)}}}{(n_2+m)!}\eta^{\beta_2^{(0)}}(2-\eta)^{-\beta_2^{(0)}}e^{-r\eta/2}[1+O(r^{-1})]$$
$$+\Delta b^{\{1\}}(-1)^{n_2+1}n_2!(2r)^{-\beta_2^{(0)}}(2-\eta)^{\beta_2^{(0)}}$$
$$\times\eta^{-\beta_2^{(0)}}e^{+r\eta/2}[1+O(r^{-1})] \,. \tag{61}$$

(Here and in the following, we use "anchored at $\eta=a$" to mean a QSC wave function generated by expansion from the point a.) If instead of starting the expansion at the boundary point $\eta=0$ we had started at $\eta=2$, exactly the same expression would have been obtained for Φ_2 anchored at $\eta=2$ ($\Phi_{2[2]}$), except that η would be replaced by $2-\eta$:

$$\Phi_{2[2]} \sim \frac{(-1)^{n_2}(2r)^{\beta_2^{(0)}}}{(n_2+m)!}$$
$$\times(2-\eta)^{\beta_2^{(0)}}\eta^{-\beta_2^{(0)}}e^{-r+r\eta/2}[1+O(r^{-1})]$$
$$+\Delta b^{\{1\}}(-1)^{n_2+1}n_2!(2r)^{-\beta_2^{(0)}}\eta^{\beta_2^{(0)}}$$
$$\times(2-\eta)^{-\beta_2^{(0)}}e^{+r-r\eta/2}[1+O(r^{-1})] \,. \tag{62}$$

These two equations represent the *same wave function* only if

$$(\Delta b^{\{1\}})^2 = \frac{(2r)^{4\beta_2^{(0)}}e^{-2r}}{[n_2!(n_2+m)!]^2}[1+O(r^{-1})] \,, \tag{63}$$

which gives the formula (54) for $\Delta b^{\{1\}}$.

The complete series for $\Delta b^{\{1\}}$ is obtained by carrying out the above process to all powers of $(2r)^{-1}$. The formal result is

$$\Delta b^{\{1\}} = \pm\frac{(2r)^{2\beta_2^{(0)}}e^{-r}}{n_2!(n_2+m)!}(\tfrac{1}{2}\phi_{[0]})^{\beta_2^{(0)}}(\tfrac{1}{2}\phi_{[2]})^{\beta_2^{(0)}}e^{-r(\phi_{[0]}+\phi_{[2]}-2)/2}\left[\frac{{}_2F_0(-n_2,-n_2-m;;-(r\phi_{[0]})^{-1})}{{}_2F_0(n_2+m+1,n_2+1;;+(r\phi_{[0]})^{-1})}\right]^{1/2}$$
$$\times\left[\frac{{}_2F_0(-n_2,-n_2-m;;-(r\phi_{[2]})^{-1})}{{}_2F_0(n_2+m+1,n_2+1;;+(r\phi_{[2]})^{-1})}\right]^{1/2} . \tag{64}$$

By $\phi_{[0]}$ is meant the ϕ for the QSC eigenfunction anchored at $\eta=0$, while $\phi_{[2]}$ corresponds to the QSC eigenfunction anchored at $\eta=2$. In fact here $\phi_{[2]}(\eta,r)=\phi_{[0]}(2-\eta,r)$. The right-hand side of Eq. (64) is $(2r)^{2\beta_2^{(0)}}e^{-r}$ times a series in $(2r)^{-1}$ that is independent of η.

The index shift $\Delta b^{\{1\}}$ and RSPT can now be put together to give the $O(e^{-r})$ contribution $\Delta\beta_2^{\{1\}}$ to β_2. Recall that in the preceding subsection (III B) the index b was set equal to $\beta_2^{(0)}$ and then the higher $\beta_2^{(N)}$ ($N\geq 1$) were obtained as functions of $\beta_2^{(0)}$ by requiring that $\phi^{(N+1)}$ vanish as $\eta\to 0$. That process did not depend on the value of $\beta_2^{(0)}$. If now $\beta_2^{(0)}\to\beta_2^{(0)}+\Delta b^{\{1\}}$, then one can expand out from the RSPT series the part linear in $\Delta b^{\{1\}}$,

$$\Delta\beta_2^{\{1\}} = \Delta b^{\{1\}}\sum_{N=0}^{\infty}\frac{d\beta_2^{(N)}}{d\beta_2^{(0)}}(2r)^{-N} \tag{65}$$
$$= \Delta b^{\{1\}}[1-4\beta_2^{(0)}(2r)^{-1}+\cdots\,] \,, \tag{66}$$

where Eq. (47) has been used to calculate $d\beta_2^{(1)}/d\beta_2^{(0)}$. In a similar way it follows that

$$\Delta\phi^{\{1\}} = \Delta b^{\{1\}}\sum_{N=0}^{\infty}\frac{d\phi^{(N)}(\eta)}{d\beta_2^{(0)}}(2r)^{-N} \tag{67}$$
$$= r^{-1}\Delta b^{\{1\}}[2\ln(1-\tfrac{1}{2}\eta)+\cdots\,] \,, \tag{68}$$

where Eq. (43) has been used to calculate $d\phi^{(1)}/d\beta_2^{(0)}$. [Note that $\phi^{(0)}$, Eq. (39), is independent of $\beta_2^{(0)}$.]

To use Eqs. (65) and (67) relating $\Delta\beta_2^{\{1\}}$ and $\Delta\phi^{\{1\}}$ to $\Delta b^{\{1\}}$, it is necessary to calculate the RSPT $\beta_2^{(N)}$ and the QSC $\phi^{(N)}$ as explicit functions of $\beta_2^{(0)}$. This is easy for low orders but tedious for high orders. An alternative procedure is given in the next subsection.

D. Solution of the Riccati equation directly to $O(e^{-r})$

To avoid solving for $\beta_2^{(N)}$ and $\phi^{(N)}$ as explicit functions of $\beta_2^{(0)}$ to high order, which would be required to use Eqs. (65) and (67) for $\Delta\beta_2^{\{1\}}$ and $\Delta\phi^{\{1\}}$, we give an alternative procedure, which is to solve the Riccati equation (35) directly to $O(e^{-r})$.

Let $q(r)$ denote the ratio

$$q(r)\equiv\Delta\beta_2^{\{1\}}/\Delta b^{\{1\}} = \sum_{N=0}^{\infty}\frac{d\beta_2^{(N)}}{d\beta_2^{(0)}}(2r)^{-N} \,. \tag{69}$$

We anticipate that $r^{-1}\Delta b^{\{1\}}$ is a natural factor in $\Delta\phi^{\{1\}}$, and we accordingly define the ratio

$$\theta(\eta,r) = \Delta\phi^{\{1\}}/r^{-1}\Delta b^{\{1\}} \,. \tag{70}$$

Let ϕ in the remainder of this section denote only the zeroth-exponential-order part of ϕ—i.e., the $1/r$ power-series part. In place of ϕ, put $\phi+r^{-1}\Delta b^{\{1\}}\theta$ into the Riccati equation (35), and put $\beta_2^{(0)}+\Delta b^{\{1\}}$ for b and $\sum\beta_2^{(N)}(2r)^{-N}+\Delta b^{\{1\}}q(r)$ for β_2. Expand the equation in powers of $\Delta b^{\{1\}}$, and keep only the terms first order in $\Delta b^{\{1\}}$. The result, divided by $r^{-1}\Delta b^{\{1\}}$, is an equation for $\theta(\eta,r)$ and $q(r)$, given $\phi(\eta,r)$:

$$\left[\frac{d\phi}{d\eta}\right]^2\left[\frac{1}{\phi}-\frac{\beta_2^{(0)}\theta}{r\phi^2}+\frac{(m^2-1)\theta}{2r^2\phi^3}\right]-2\frac{d\phi}{d\eta}\frac{d\theta}{d\eta}\left[\frac{1}{4}-\frac{\beta_2^{(0)}}{r\phi}+\frac{m^2-1}{4r^2\phi^2}\right]-q(r)\left[\frac{1}{\eta}+\frac{1}{2-\eta}\right]$$
$$-\frac{1}{2r^2}\frac{d\theta}{d\eta}\left[\frac{d\phi}{d\eta}\right]^{-1/2}\frac{d^2}{d\eta^2}\left[\frac{d\phi}{d\eta}\right]^{-1/2}+\frac{1}{2r^2}\left[\frac{d\phi}{d\eta}\right]^{1/2}\frac{d^2}{d\eta^2}\left[\frac{d\theta}{d\eta}\left[\frac{d\phi}{d\eta}\right]^{-3/2}\right]=0\ . \qquad (71)$$

To solve Eq. (71), first expand $q(r)$ and $\theta(\eta,r)$ in power series in $(2r)^{-1}$:

$$q(r)=\sum_{N=0}^{\infty} q^{(N)}(2r)^{-N}\ , \qquad (72)$$

$$\theta(\eta,r)=\sum_{N=0}^{\infty}\theta^{(N)}(\eta)(2r)^{-N}\ . \qquad (73)$$

From Eq. (71) and $\phi^{(0)}$ [Eq. (39)], one obtains the zeroth-order equation,

$$\tfrac{1}{2}d\theta^{(0)}/d\eta=\eta^{-1}-q^{(0)}[\eta^{-1}+(2-\eta)^{-1}]\ . \qquad (74)$$

Since $d\theta^{(0)}/d\eta$ must be finite at $\eta=0$,

$$q^{(0)}=1,\quad \theta^{(0)}=2\ln(1-\tfrac{1}{2}\eta)\ . \qquad (75)$$

Similarly, one obtains the equation

$$d\theta^{(1)}/d\eta=(d/d\eta)[16\beta_2^{(0)}\eta^{-1}\ln(1-\tfrac{1}{2}\eta)]$$
$$-8\beta_2^{(0)}(2-\eta)^{-2}$$
$$-2(4\beta_2^{(0)}+q^{(1)})[\eta^{-1}+(2-\eta)^{-1}]\ . \qquad (76)$$

From the regularity condition at $\eta=0$ it follows that

$$q^{(1)}=-4\beta_2^{(0)}\ , \qquad (77)$$

$$\theta^{(1)}=16\beta_2^{(0)}[\eta^{-1}\ln(1-\tfrac{1}{2}\eta)+\tfrac{1}{2}]$$
$$-8\beta_2^{(0)}[(2-\eta)^{-1}-\tfrac{1}{2}]\ . \qquad (78)$$

Thus the ratios $q(r)$ and $\theta(\eta,r)$ can be calculated by a recursive, perturbative technique directly, rather than through the $\beta_2^{(0)}$ derivatives of the $\phi^{(n)}$ and the $\beta_2^{(N)}$. It is interesting that there is yet another alternative method for calculating $q(r)$—a "normalization-integral" method—that will be given in the next subsection.

E. Normalization-integral formula for $q(r)$

The two methods given previously for $q(r)$ are generalizable to higher exponential orders. A third formula is developed in this section that is less generalizable but simpler in the respect that it uses only the zeroth-exponential-order wave function in the practical evaluation of $q(r)$. The argument starts out with a "current-density" formula and ends up with an expression that looks like a normalization integral.

Let $\Phi^{(+)}$ and $\Phi^{(-)}$ denote the paired solutions of Eq. (11) that differ only in the choice of sign for $\Delta b^{\{1\}}$ in Eq. (64). To $O(e^{-r})$ the difference in the two eigenvalues—i.e., the double-well gap for these two states—is $2\Delta\beta_2^{\{1\}}$. From Eq. (11) one sees by a standard current-density argument that

$$2\Delta\beta_2^{\{1\}}+O(e^{-2r})=\frac{\Phi^{(+)}(d\Phi^{(-)}/d\eta)-\Phi^{(-)}(d\Phi^{(+)}/d\eta)}{r\int_0^{\eta}\Phi^{(+)}\Phi^{(-)}[\eta^{-1}+(2-\eta)^{-1}]d\eta}\ . \qquad (79)$$

The numerator is a Wronskian of two functions that solve the same differential equation if terms $O(r^k e^{-r})$ are neglected. From the form of $\Phi^{(\pm)}$ [in terms of the Whittaker M function, Eq. (34)], from Eqs. (55) and (56) [or more simply Eq. (57)] for the asymptotics of the M function, from the Wronksian of the Whittaker functions,[20]

$$W_{b,m/2}(z)\frac{d}{dz}e^{\mp\pi i b}W_{-b,m/2}(ze^{\mp\pi i})$$
$$-e^{\mp\pi i b}W_{-b,m/2}(ze^{\mp\pi i})\frac{d}{dz}W_{b,m/2}(z)=1\ , \qquad (80)$$

and from standard error estimates for formulas of this type,[4] it follows that so long as $0\ll\eta\ll 2$, i.e., for $\eta=1+\epsilon$ ($\epsilon\sim 0$), the numerator is to first exponential order,

$$2rn_2!\Delta b^{\{1\}}/(n_2+m)!\ . \qquad (81)$$

Similarly, also for $0\ll\eta\ll 2$, the denominator is to terms $O(r^k e^{-r})$ independent of η and dominated by the exponentially decreasing component, the $W_{b,m/2}$ in Eq. (55). Since for $b=\beta_2^{(0)}$ this W is just an unperturbed wave function, there is no difficulty and insignificant error in replacing the M by the unperturbed W, expanding the integrand as $e^{-r\eta}$ times a power series in $(2r)^{-1}$ and in η, and then taking the upper limit of the integral to be ∞. That is, the denominator is again up to $O(r^k e^{-r})$

$$r[(n_2+m)!]^{-2}\int_0^{\infty}(d\phi/d\eta)^{-1}[W_{\beta_2^{(0)},m/2}(r\phi)]^2$$
$$\times[\eta^{-1}+(2-\eta)^{-1}]d\eta\ . \qquad (82)$$

We emphasize that (82) is not meant literally, but instead as an asymptotic power series in $(2r)^{-1}$. Also, ϕ is meant to be the zeroth-exponential-order solution of the Riccati equation (35). Thus one obtains for $q(r)=\Delta\beta_2^{\{1\}}/\Delta b^{\{1\}}$,

$$q(r)=n_2!(n_2+m)!\left[\int_0^{\infty}(d\phi/d\eta)^{-1}[W_{\beta_2^{(0)},m/2}(r\phi)]^2\times[\eta^{-1}+(2-\eta)^{-1}]d\eta\right]^{-1}\ . \qquad (83)$$

Equation (83), being only an integral to be evaluated, is perhaps the most useful practical expression for computing $q(r)$.

F. Imaginary contribution to the index b

As mentioned in the Introduction and in Sec. II C, same-sign factorial divergence suggests a complex, discontinuous Borel sum [cf. Eqs. (3) and (4)]. For the RSPT for β_2, we infer from Eq. (28) that for the ground state, with $r>0$,

$$\sum_{N=0}^{\infty} \beta_2^{(N)}(2r)^{-N} \sim -\sum_{N=0}^{\infty}(N+1)!(2r)^{-N} \tag{84}$$

$$\sim \mathrm{P}\int_0^{\infty} t^2 e^{-t}(t-2r)^{-1}dt \pm i\pi 4r^2 e^{-2r} \quad (\mathrm{Im}\, r=\pm 0)\ . \tag{85}$$

This motivates us to look for an *explicit* contribution to β_2 that is $O(e^{-2r})$ and that is *imaginary*, to cancel the imaginary term in Eq. (85).

Since the Riccati equation (35) is formally real, explicit imaginary terms in β_2 can only originate in the index b. The value of b through $O(e^{-r})$ was obtained in Sec. III C by matching two QSC wave functions that separately satisfied the boundary conditions at either $\eta=0$ or 2, and that value was real (for real r and η). The imaginary $O(e^{-2r})$ contribution has its computational origin in the complex phase factor multiplying the subdominant contribution to the ordinary asymptotic expansion for the Whittaker M function, Eqs. (55) and (56).

The reader is well aware that the Whittaker M function is real on the real axis, and that the complex expansion (56) is not usually considered valid[21] on the real axis, which is a Stokes line of the expansion.[21] However, there is a sense[7] in which the complex expansion (56) is valid also on the real axis. In fact, the two power-series expansions represented by the $_2F_0$ functions in Eq. (56) are Borel summable,[7] and the overall result is the Whittaker M function in each appropriate half-plane. The positive real axis is a cut of the Borel sum of the power series multiplying $e^{+z/2}$, the dominant expansion. In the limit as $\mathrm{Im}\, z \rightarrow 0$ from above or below, the imaginary part of the Borel sum times $e^{+z/2}$ cancels the explicit imaginary contribution coming from the phase factor multiplying the subdominant expansion. This is the sense in which the sum of the explicitly complex, discontinuous expansion mentioned in the Introduction is real and continuous. The same phenomenon that holds for the Whittaker M function appears to apply to β_2. (See Ref. 6 for a proof that the Borel sum of the RSPT series for β_2 is complex.)

Let us now get on with the details of extending the matching process of Sec. III C to $O(e^{-2r})$. First we extend the notation to include second exponential order [cf. Eqs. (51)—(53)]:

$$\beta_i \sim \sum_{N=0}^{\infty} \beta_i^{(N)}(2r)^{-N} + \Delta\beta_i^{\{1\}} + \Delta\beta_i^{\{2\}} + O(r^k e^{-3r}) \quad (i=1,2)\ , \tag{86}$$

$$b \sim \beta_2^{(0)} + \Delta b^{\{1\}} + \Delta b^{\{2\}} + O(r^k e^{-3r})\ , \tag{87}$$

$$\phi(\eta,r) \sim \sum_{N=0}^{\infty} \phi^{(N)}(\eta)(2r)^{-N} + \Delta\phi^{\{1\}} + \Delta\phi^{\{2\}} + O(r^k e^{-3r})\ . \tag{88}$$

Next we keep the phase factor in Eqs. (55)—(57) and get as a requirement for the matching of the two QSC functions, instead of Eqs. (64) and (63),

$$(\Delta b^{\{1\}} + \Delta b^{\{2\}})^2 = e^{\mp 2\pi i \Delta b^{\{1\}}} \times [\text{right-hand side of Eq. (64)}]^2 \times [1 + O(\Delta b^{\{1\}})] \tag{89}$$

$$= e^{\mp 2\pi i \Delta b^{\{1\}}} \frac{(2r)^{4\beta_2^{(0)}} e^{-2r}}{[n_2!(n_2+m)!]^2}[1+O(r^{-1})] \quad (\pm \mathrm{Im}\, r \geq 0)\ . \tag{90}$$

(The $O(\Delta b^{\{1\}})$ error in Eq. (89) comes from replacing the $\Gamma(\frac{1}{2}m+\frac{1}{2}\pm b)$ [cf. Eq. (55)] by $(n_2+m)!$ and $n_2!$. There is no contribution from this term to $\mathrm{Im}\Delta b^{\{2\}}$ (this section), but there is a contribution to $\mathrm{Re}\Delta b^{\{2\}}$ that will be taken care of in Sec. III H.)

The imaginary contribution to $\Delta b^{\{2\}}$ comes from the expansion of the phase factor. Take the square root of both sides of Eq. (89), then expand the factor $e^{\mp \pi i \Delta b^{\{1\}}}$:

$$\Delta b^{\{1\}} + \Delta b^{\{2\}} = (1 \mp i\pi\Delta b^{\{1\}}) \times [\text{right-hand side of Eq. (64)}] \times [1 + O(\Delta b^{\{1\}})] \tag{91}$$

$$= (1 \mp i\pi\Delta b^{\{1\}}) \times \Delta b^{\{1\}} \times [1 + O(\Delta b^{\{1\}})]\ . \tag{92}$$

Let $\Delta_r b^{\{2\}}$ and $\Delta_i b^{\{2\}}$ denote the real and imaginary parts of $\Delta b^{\{2\}}$ when r is real and positive, and their analytic continuations otherwise:

$$\Delta b^{\{2\}} = \Delta_r b^{\{2\}} + i\Delta_i b^{\{2\}}\ . \tag{93}$$

Then it is immediately seen from Eq. (92) that the second-exponential-order imaginary contribution to b is

$$\Delta_i b^{\{2\}} = \mp\pi(\Delta b^{\{1\}})^2 \quad (\pm \mathrm{Im}\, r \geq 0)\ . \tag{94}$$

This relationship between the asymptotic expansions is exact. It is the key to the Brézin—Zinn-Justin conjecture[12] discussed in the next subsection. Note, moreover, that for the ground state,

$$\Delta_i b^{\{2\}} \sim \mp\pi 4r^2 e^{-2r} \quad (\mathrm{Im}\, r=\pm 0)\ , \tag{95}$$

so that $i\Delta_i b^{\{2\}}$ to leading order is exactly the counterterm to cancel the imaginary part of Eq. (85).

G. Imaginary contribution to β_2. The gap-squared formula

The imaginary series (94) contributing to the index b leads directly to an imaginary series in β_2 that is $O(e^{-2r})$. Denote by $\Delta_r\beta_2^{\{2\}}$ and $\Delta_i\beta_2^{\{2\}}$ the real and imaginary series contributing to $\Delta\beta_2^{\{2\}}$ when r is real and positive:

$$\Delta\beta_2^{\{2\}}=\Delta_r\beta_2^{\{2\}}+i\Delta_i\beta_2^{\{2\}} . \tag{96}$$

By exactly the same argument that led to Eq. (65) for $\Delta\beta_2^{\{1\}}$, one finds that the imaginary series to second exponential order is obtained from $\Delta_i b^{\{2\}}$ via

$$\Delta_i\beta_2^{\{2\}}=\Delta_i b^{\{2\}}\sum_{N=0}^{\infty}\frac{d\beta_2^{(N)}}{d\beta_2^{(0)}}(2r)^{-N} \tag{97}$$

$$=\Delta_i b^{\{2\}}q(r) \tag{98}$$

$$=\mp\pi\frac{(2r)^{4\beta_2^{(0)}}e^{-2r}}{[n_2!(n_2+m)!]^2}[1+O(r^{-1})] \quad (\pm\mathrm{Im}r\geq 0) . \tag{99}$$

The importance of $\Delta_i\beta_2^{\{2\}}$ is the role it plays, via a dispersion relation[6] to be discussed later in Sec. VI, in the asymptotics of the RSPT coefficients $\beta_2^{(N)}$:

$$\beta_2^{(N)}\sim\pi^{-1}2^N\int_0^{\infty+i\epsilon}r^{N-1}\Delta_i\beta_2^{\{2\}}dr . \tag{100}$$

The $\infty+i\epsilon$ is to indicate that the "$\mathrm{Im}r\geq 0$ sign" is to be used for $\Delta_i b^{\{2\}}$ in Eq. (94). Since the same ratio $q(r)$ occurs here that occurred for the first-exponential-order quantity $\Delta\beta_2^{\{1\}}$ [Eqs. (66)–(69)], it is possible to express $\Delta_i\beta_2^{\{2\}}$ directly in terms of $\Delta\beta_2^{\{1\}}$ and $q(r)$ via Eq. (94):

$$\Delta_i\beta_2^{\{2\}}=\mp\pi(\Delta\beta_2^{\{1\}})^2/q(r) \quad (\pm\mathrm{Im}r\geq 0) , \tag{101}$$

which, because of Eq. (83), can be written as the product of $\mp\pi$, the "half gap" squared, and a normalization integral, taken in the sense of an asymptotic power series as explained in Sec. III E,

$$\Delta_i\beta_2^{\{2\}}=\mp\pi(\Delta\beta_2^{\{1\}})^2\frac{\int_0^{\infty}(d\phi/d\eta)^{-1}[W_{\beta_2^{(0)},m/2}(r\phi)]^2[\eta^{-1}+(2-\eta)^{-1}]d\eta}{n_2!(n_2+m)!} \quad (\pm\mathrm{Im}r\geq 0) . \tag{102}$$

Recall that the expansion for $q(r)$ starts out with 1 [cf. Eqs. (66) and (75)]. Equations (101) and (102) express the *exact* relationship between the asymptotics of the $\beta_2^{(N)}$ [via Eq. (100)] and the square of the gap whose leading term was found numerically by Brézin and Zinn-Justin.[9] In fact, that relationship did not involve β_2 but the energy $E(R)$. It will be seen in Sec. VI, however, that the asymptotics of the $E^{(N)}$ are dominated by $\Delta_i\beta_2^{\{2\}}$, so that the crux of the explanation of the $E^{(N)}$ asymptotics has already been given.

H. Doubly-exponentially-small real series

The matching process described in Sec. III C was carried out there to $O(e^{-r})$ for the index shift $\Delta b^{\{1\}}$ and in Sec. III F for the $O(e^{-2r})$ imaginary shift $\Delta_i b^{\{2\}}$. In this section the calculation of the shift in b to any exponential order is sketched, and results are given for the real $O(e^{-2r})$ shift $\Delta_r b^{\{2\}}$ and the real second-exponential-order $\Delta_r\beta_2^{\{2\}}$.

The formulas in this section involve the logarithmic derivative of the gamma function,[19] usually defined by ψ:

$$\psi(z)=\frac{d}{dz}\ln\Gamma(z) . \tag{103}$$

The exact form of the matching equation that results from equating the two QSC functions, one anchored at $\eta=0$, the other at $\eta=2$, the $O(e^{-r})$ version of which is Eq. (64), is [cf. Eqs. (34) and (55)–(59)]

$$b=\beta_2^{(0)}+\Delta b , \tag{104}$$

$$\pi^{-2}\sin^2(\pi\Delta b)=\frac{e^{\mp 2\pi i\Delta b}}{[\Gamma(n_2+m+1+\Delta b)\Gamma(n_2+1+\Delta b)]^2}\frac{W_{\beta_2^{(0)}+\Delta b,m/2}(r\phi_{[0]})}{e^{\mp\pi i(\beta_2^{(0)}+\Delta b)}W_{-\beta_2^{(0)}-\Delta b,m/2}(r\phi_{[0]}e^{\mp\pi i})}\times\frac{W_{\beta_2^{(0)}+\Delta b,m/2}(r\phi_{[2]})}{e^{\mp\pi i(\beta_2^{(0)}+\Delta b)}W_{-\beta_2^{(0)}-\Delta b,m/2}(r\phi_{[2]}e^{\mp\pi i})} \quad (\pm\mathrm{Im}r\geq 0) . \tag{105}$$

As with Eq. (64), the η dependence of the right-hand side of Eq. (105) cancels, leaving only a function of r. Now expand Δb in exponentially ordered terms $\Delta b^{\{q\}}$,

$$\Delta b=\sum_{q=1}^{\infty}\Delta b^{\{q\}} . \tag{106}$$

The asymptotic equation for Δb, which is the general version of Eq. (64) valid to all exponential orders, is obtained by using the asymptotic expansions [cf. Eqs. (55)–(57)] for the Whittaker functions and taking the square root of both sides of Eq. (105). To put the result in a form that can be solved recursively for the $\Delta b^{\{q\}}$ after expansion, we add $\pi^{-1}\sin(\pi\Delta b)-\Delta b$ to both sides (after taking the square root). Then for $\mathrm{Im}r\geq 0$ (the complex conjugate holds for the reverse) we obtain

$$\Delta b=-[\pi^{-1}\sin(\pi\Delta b)-\Delta b]\pm\frac{e^{-\pi i\Delta b}(2r)^{2\beta_2^{(0)}+2\Delta b}e^{-r}}{\Gamma(n_2+m+1+\Delta b)\Gamma(n_2+1+\Delta b)}(\tfrac{1}{2}\phi_{[0]})^{\beta_2^{(0)}+\Delta b}(\tfrac{1}{2}\phi_{[2]})^{\beta_2^{(0)}+\Delta b}e^{-r(\phi_{[0]}+\phi_{[2]}-2)/2}$$
$$\times\left[\frac{{}_2F_0(-n_2-\Delta b,-n_2-m-\Delta b;;-(r\phi_{[0]})^{-1})}{{}_2F_0(n_2+m+1+\Delta b,n_2+1+\Delta b;;+(r\phi_{[0]})^{-1})}\right]^{1/2}$$
$$\times\left[\frac{{}_2F_0(-n_2-\Delta b,-n_2-m-\Delta b;;-(r\phi_{[2]})^{-1})}{{}_2F_0(n_2+m+1+\Delta b,n_2+1+\Delta b;;+(r\phi_{[2]})^{-1})}\right]^{1/2} . \quad (107)$$

The leading term of the second-exponential-order real series comes from the expansion of the Γ functions and of $(2r)^{2\Delta b}$, the latter of which leads to $\ln(2r)$ terms. Subsequent terms are down by $1/2r$ and require ϕ through $O(e^{-r})$. Like $\Delta_i b^{\{2\}}$, the real $\Delta_r b^{\{2\}}$ is proportional to the square of the first-exponential-order series. The first few terms of $\Delta_r b^{\{2\}}$ are

$$\Delta_r b^{\{2\}}=(\Delta b^{\{1\}})^2[2\ln(2r)-\psi(n_2+1)-\psi(n_2+m+1)-12\beta_2^{(0)}(2r)^{-1}+O(r^{-2})] . \quad (108)$$

The real second-exponential-order contribution $\Delta_r\beta_2^{\{2\}}$ to β_2 can be found from the index shift as in Sec. III C, Eq. (65), except that now second derivatives with respect to $\beta_2^{(0)}$ are required:

$$\Delta\beta_2^{\{2\}}=\Delta b^{\{2\}}\sum_{N=0}^{\infty}\frac{d\beta_2^{(N)}}{d\beta_2^{(0)}}(2r)^{-N}+\tfrac{1}{2}(\Delta b^{\{1\}})^2\sum_{N=1}^{\infty}\frac{d^2\beta_2^{(N)}}{d(\beta_2^{(0)})^2}(2r)^{-N} . \quad (109)$$

As for the first-exponential-order case in Sec. III D, it is also possible to avoid the second derivatives of the $\beta_2^{(N)}$ by solving the Riccati equation directly to second exponential order, but we omit the details here. The leading terms in the expansion for $\Delta_r\beta_2^{\{2\}}$ are

$$\Delta_r\beta_2^{(2)}=\frac{(2r)^{4\beta_2^{(0)}}e^{-2r}}{(n_2!)^2[(n_2+1)!]^2}\Bigg[2\ln(2r)-\psi(n_2+1)-\psi(n_2+m+1)$$
$$+\frac{1}{2r}\Big[[2\ln(2r)-\psi(n_2+1)-\psi(n_2+m+1)]$$
$$\times[-4\beta_2^{(0)}-12(\beta_2^{(0)})^2+m^2-1]-12\beta_2^{(0)}-2\Big]+O(r^{-2}\ln(2r))\Bigg] . \quad (110)$$

I. The β_2 equation on a semi-infinite interval and the discontinuity in the Borel sum

In this section we treat a different problem: we solve the β_2 eigenvalue equation not on the original finite interval, but on a semi-infinite interval. There are two reasons for considering this modified problem. (i) It has the same RSPT expansion as the original problem, but the Borel sum of the common RSPT expansion *is* the eigenvalue of this modified problem.[5,6] (ii) The positive r axis is a cut of the eigenvalue of the modified problem, and calculation of the discontinuity across the cut gives an immediate, unambiguous meaning to the imaginary second-exponential-order series $\Delta_i\beta_2^{(2)}$ calculated already in Sec. III G, but which comes up again here: it is the discontinuity that determines the dispersion relation and that gives the asymptotics of the RSPT coefficients [cf. Eq. (100) and Sec. VI].

The problem is to solve Eq. (11) with the boundary conditions

$$\Phi_2(\eta)\to 0 \text{ as } \eta\to 0 \text{ and as } \mathrm{Re}(\eta r)\to+\infty,\ \mathrm{Im}(\eta r)>0 \quad (111)$$

or equivalently Eq. (16) with the boundary conditions

$$\Phi_2(v)\to 0 \text{ as } v\to 0 \text{ and as } \mathrm{Re}v\to+\infty,\ \mathrm{Im}r>0 . \quad (112)$$

The nonstandard aspect of this modified problem is to avoid the singularity on the positive real axis at $\eta=2$ for Eq. (11) or at $v=2r$ for Eq. (16), as indicated by the $\mathrm{Im}r>0$ in Eq. (112). The modified eigenvalue problem is related to a standard eigenvalue problem: the ξ (or u) equation when the Schrödinger equation for an electron moving in the field of a proton and an antiproton [change the sign of the $1/r_b$ term in Eq. (9)] is separated in prolate spheroidal coordinates. The u equation is

$$[-u\,d^2/du^2+\tfrac{1}{4}u+\tfrac{1}{4}(m^2-1)/u]\Phi_1'+uV_1'(u,\beta_1',r')\Phi_1'=\beta_1'\Phi_1' , \quad (113)$$

$$V_1'(u,\beta_1',r')=+\frac{\beta_1'}{2r'+u}+\tfrac{1}{4}(m^2-1)\left[-\frac{2}{u(2r'+u)}\frac{1}{(2r'+u)^2}\right] \quad (0\le u<\infty) , \quad (114)$$

where the primes are to distinguish the mixed-charge problem from H_2^+. The modified β_2 problem is the analytic continuation up to $r'=e^{\pm\pi i}r$ of the stable, single-well β_1' problem. (See Sec. IV of Ref. 6 for the use of this approach in estimating rigorously the leading term in the discontinuity.)

Before giving the details of the QSC solution, one can anticipate certain of its characteristics, which depend on how the singularity on the positive v or η axis is avoided. The v case is easier to state but completely equivalent to the η case. By making r complex, the singularity at $v=2r$ [see Eq. (21)] is moved off the positive axis. Note[5,6] that the positive r axis is a cut for $\beta_1'(r)$, where $r'=e^{\pm\pi i}r$. If $\mathrm{Im}\,r>0$, then the direct Borel sum [for which $|\arg(r')|<\pi$] of the RSPT series will be $\beta_1'(e^{-\pi i}r)$, while if $\mathrm{Im}\,r<0$, the direct Borel sum will be $\beta_1'(e^{+\pi i}r)$. Now here is the subtlety: suppose one requires the complete asymptotic expansion for $\beta_1'(e^{-\pi i}r)$ both for $\mathrm{Im}\,r>0$, where the answer has to be exactly RSPT, and for its *analytic continuation to* $\mathrm{Im}\,r<0$, where the answer cannot be exactly RSPT, because for $\mathrm{Im}\,r<0$ the Borel sum of the RSPT series is $\beta_1'(e^{+\pi i}r)$. In the fourth quadrant, the asymptotic expansion for $\beta_1'(e^{-\pi i}r)$ necessarily must have, besides the RSPT terms, additional terms that represent the difference, $\beta_1'(e^{-\pi i}r)-\beta_1'(e^{+\pi i}r)$, below the positive real r axis. In other words, these additional terms represent the discontinuity in the eigenvalue of the modified problem across the cut on the positive r axis.

The major difference in the details for the modified problem versus the original β_2 problem is the choice of Whittaker function for the solution anchored at $\eta=2$. In the original case the choice was an M function to be regular at $\eta=2$. In the present case the solution does not have to be regular at $\eta=2$: instead it must vanish as $\eta\to\infty$. For $\mathrm{Im}\,r>0$, the correct choice for Φ_2 anchored at $\eta=2$ [$\Phi_{2[2]}$] which vanishes at infinity [cf. Eqs. (55)–(57)] is $W_{-b,m/2}(e^{-\pi i}z)$:

$$\Phi_{2[2]}=(-d\phi_{[2]}/d\eta)^{-1/2}e^{-\pi i b}W_{-b,m/2}(e^{-\pi i}r\phi_{[2]}) \quad (\mathrm{Im}\,r>0)\,. \tag{115}$$

The details of the calculation of both $\phi_{[0]}$ and $\phi_{[2]}$ are exactly the same as before. Only the value of the index b needs clarification.

The index b must be chosen to make the two QSC wave functions the same. The asymptotic behavior for the QSC function anchored at $\eta=0$ is given by Eq. (61). It always has a term with a negative exponential factor $e^{-r\eta/2}$. If the index shift $\Delta b\neq 0$, it will also have a term with a positive exponential factor $e^{+r\eta/2}$. The QSC wave function anchored at $\eta=2$ in the present case has only a negative exponential factor:

$$\Phi_{2[2]}\sim(-d\phi_{[2]}/d\eta)^{-1/2}(r\phi_{[2]})^{-b}e^{+r\phi_{[2]}/2}\times{}_2F_0(\tfrac{1}{2}m+\tfrac{1}{2}+b,\tfrac{1}{2}-\tfrac{1}{2}m+b;;+(r\phi_{[2]})^{-1}) \tag{116}$$

$$\sim(2r)^{-b}\eta^{b}(2-\eta)^{-b}e^{r-r\eta/2}[1+O(r^{-1})]\,. \tag{117}$$

Comparison of Eq. (117) with Eq. (61) shows that the two solutions can be identical (except for normalization) only if $\Delta b\equiv 0$, in which case the solution anchored at $\eta=0$ has no positive exponential factor, and $b=\beta_2^{(0)}$. Thus when $\mathrm{Im}\,r>0$, there is no additional, exponentially small contribution to the expansion for β_2 for the modified problem, i.e., $\beta_1'(e^{-\pi i}r)$, as has been shown rigorously.[5,6]

Now consider the analytic continuation of the QSC function based on the Whittaker $W_{-b,m/2}$, across the positive real axis to $\mathrm{Im}\,r<0$. Since $\arg(e^{-\pi i}r)<-\pi$ when $\arg(r)$ is negative, the asymptotic expansion (116) is no longer valid. To get the correct expansion for the Whittaker function the argument of the $r\phi_{[2]}$ must first be brought within the range $(-\pi,\pi)$ by the circuital relation[20]

$$e^{-\pi i b}W_{-b,m/2}(e^{-\pi i}r\phi_{[2]})=e^{+\pi i b}W_{-b,m/2}(e^{+\pi i}r\phi_{[2]})-\frac{2\pi i W_{b,m/2}(r\phi_{[2]})}{\Gamma(b+\frac{1}{2}+\frac{1}{2}m)\Gamma(b+\frac{1}{2}-\frac{1}{2}m)} \tag{118}$$

$$\sim(2r)^{-b}\eta^{-b}(2-\eta)^{-b}e^{r-r\eta/2}-\frac{2\pi i}{(n_2+m)!n_2!}(2r)^{b}\eta^{-b}(2-\eta)^{b}e^{-r+r\eta/2}\,. \tag{119}$$

Since both exponentials now appear, they must also appear in the M-based QSC function anchored at $\eta=0$. Consequently Δb cannot vanish. The exact matching equation to determine Δb, the analog of Eq. (105), is

$$\pi^{-1}\sin(\pi\Delta b)=\frac{2\pi i e^{+\pi i\Delta b}}{[\Gamma(n_2+m+1+\Delta b)\Gamma(n_2+1+\Delta b)]^2}\,\frac{W_{\beta_2^{(0)}+\Delta b,m/2}(r\phi_{[0]})}{e^{+\pi i(\beta_2^{(0)}+\Delta b)}W_{-\beta_2^{(0)}-\Delta b,m/2}(r\phi_{[0]}e^{+\pi i})}\times\frac{W_{\beta_2^{(0)}+\Delta b,m/2}(r\phi_{[2]})}{e^{+\pi i(\beta_2^{(0)}+\Delta b)}W_{-\beta_2^{(0)}-\Delta b,m/2}(r\phi_{[2]}e^{+\pi i})}\quad(\mathrm{Im}\,r<0)\,. \tag{120}$$

[Note that even though Eq. (120) appears to be η dependent, as before the η dependence cancels out, and Δb depends only on r.]

Compare the matching formula here [Eq. (120)] with Eq. (105). It is easily seen that the lowest nonvanishing exponential order of the right-hand side of Eq. (120) is the second, that it is purely imaginary, and that it is $2\pi i$ times the square of the previously determined half-gap index shift $\Delta b^{\{1\}}$ of Eqs. (63) and (64):

$$\Delta b(\text{modified }\beta_2\text{ equation})=+2\pi i(\Delta b^{\{1\}})^2+O(r^k e^{-4r})\quad(\mathrm{Im}\,r<0,\ \arg r'<-\pi) \tag{121}$$

$$=2i\Delta_i b^{\{2\}}+O(r^k e^{-4r})\quad(\mathrm{Im}\,r<0,\ \arg r'<-\pi)\,. \tag{122}$$

Thus the index shift on analytic continuation from the first to the fourth quadrant is nonvanishing in second exponential order and is exactly 2 times the second-exponential-order imaginary index shift already calculated for the original β_2 problem. Since the mechanism by which the lowest-order nonvanishing imaginary index shift induces an imaginary contribution to β_2 is exactly the same for both the original and modified problems, Eqs. (97)—(102), a second-exponential-order contribution completely analogous to Eq. (122) holds for the modified β_2:

$$\beta_1'(e^{-\pi i}r) \sim \sum_{N=0}^{\infty} \beta_2^{(0)}(2r)^{-N} + 2i\Delta_i\beta_2^{\{2\}} + O(r^k e^{-4r})$$
$$(\operatorname{Im} r < 0,\ \arg r' < -\pi)\ . \quad (123)$$

As anticipated, by analytic continuation directly across the positive r axis, one finds a purely imaginary $O(e^{-2r})$ series in addition to the RSPT series. At the real axis, this series represents to lowest exponential order the discontinuity at the cut of the Borel sum of the RSPT series,

$$\beta_1'(e^{-\pi i}r) - \beta_1'(e^{+\pi i}r) \sim 2\pi i(\Delta b^{\{1\}})^2 q(r)\ , \quad (124)$$

and as such is the dominating factor in the dispersion relation that gives the asymptotic behavior of the RSPT coefficients, to be discussed further in Sec. VI. Since the RSPT series coefficients are real and the discontinuity is purely imaginary, the imaginary parts of the Borel sums just above and below the positive real axis are equal in magnitude and opposite in sign:

$$\operatorname{Im}\left[\lim_{\operatorname{Im} r \to \pm 0}\left[\text{Borel sum of } \sum \beta_2^{(N)}(2r)^{-N}\right]\right]$$
$$\sim \pm\pi(\Delta b^{\{1\}})^2 q(r)\ . \quad (125)$$

The explicit imaginary series found for the original β_2 problem [Eqs. (94)—(102)] is exactly this result (125), but with opposite sign. This clearly demonstrates the cancellation of the explicit imaginary second-exponential-order series with the implicit imaginary part of the Borel sum of the double-well problem, the phenomenon of a complex expansion with a real sum, mentioned in the Introduction.

IV. THE β_1 EQUATION

Although most of the interesting results for $H_2{}^+$ come from the β_2 equation, yet the β_1 equation adds its own distinctive twist in the form of a branch cut in the *negative* r direction and in the form of logarithmic terms.[22] Both $\beta_1^{(N)}$ and $E^{(N)}$ get asymptotic contributions with *alternating signs* and with a $\ln N$ dependence, but the relative magnitudes with respect to the dominant, same-sign behavior are down by several powers of N.

Before discussing these unique contributions, we dispense first with the terms in β_1 that are "induced" by the exponentially small terms $\Delta\beta_2 = \Delta\beta_2^{\{1\}} + \Delta\beta_2^{\{2\}} + \cdots$ already in β_2. Consider $\Delta\beta_2$ to be a shift of $\beta_2^{(0)}$. Then the induced effect on $\Delta\beta_1$ is expressed by the Taylor series

$$(\Delta\beta_1)_{\text{ind}} = \sum_{k=1}^{\infty} \frac{(\Delta\beta_2)^k}{k!} \left[\frac{\partial}{\partial\beta_2^{(0)}}\right]^k \sum_{N=0}^{\infty} \beta_1^{(N)}(2r)^{-N}\ . \quad (126)$$

The dependence of $\beta_1^{(N)}$ on $\beta_2^{(0)}$ is determined through Eqs. (15) and (18)—(20). The use of partial derivatives in Eq. (126) is to indicate that the $\beta_2^{(N)}$ $(N \geq 1)$ are to be held constant. An alternative method to obtain $(\Delta\beta_1)_{\text{ind}}$ is to regard the terms $-2u(u+2r)^{-1}(\Delta\beta_2^{\{1\}} + \Delta\beta_2^{\{2\}} + \cdots)$ in Eq. (18) as a second, independent perturbation. The effect on $\Delta\beta_1$ can then be calculated by double RSPT. In particular, the leading real first-exponential-order series and the leading imaginary second-exponential-order series, $\Delta\beta_1^{\{1\}}$ and $i\Delta_i\beta_1^{\{2\}}$, can be obtained by the standard perturbation formula first order in the exponentially small perturbation but infinite order in the $1/r$ perturbation. That is, with the ordinary RSPT wave function for Φ_1 in powers of $(2r)^{-1}$, Φ_{RSPT}, the induced exponentially small contributions to β_1 in leading exponential order are

$$(\Delta\beta_1^{\{1\}} + i\Delta_i\beta_1^{\{2\}})_{\text{ind}} = \frac{-2(\Delta\beta_2^{\{1\}} + i\Delta_i\beta_2^{\{2\}}) \int_0^\infty \Phi_{\text{RSPT}}^2 (u+2r)^{-1} du}{\int_0^\infty \Phi_{\text{RSPT}}^2 [u^{-1} + (u+2r)^{-1}] du}\ . \quad (127)$$

Here Φ_{RSPT} refers to the solution of Eq. (15) by RSPT in powers of $(2r)^{-1}$. Both integrals are to be evaluated order by order in powers of $(2r)^{-1}$. In short, the induced exponentially small contributions to β_1 are straightforward to obtain but are otherwise unremarkable.

The more interesting exponentially small contributions to β_1 come from a cut in the negative r direction, which is suggested by the singularity in Eq. (15) [cf. also Eq. (18)] at $u = -2r$. Associated with this cut is a dispersion relation that implies alternating-sign asymptotic contributions to $\beta_1^{(N)}$ and to $E^{(N)}$, both proportional to $(N - 4n_2 - 3m - 5)!$ [which is $(n_2 + 4m + 6)$ powers of N down from the asymptotics of the $\beta_2^{(N)}$].

One obtains an explicit formula for the discontinuity in β_1 across the cut by connecting a QSC wave function anchored at the origin, which we denote by $\Phi_{[0]}$, with one with the correct behavior at infinity, but that is anchored at $u = -2r$, which we denote by $\Phi_{[-2]}$. As in the semi-infinite treatment of the β_2 equation in Sec. III I, the role of the QSC function anchored at a singularity that is not an endpoint is to provide control of analytic continuation around that singularity. As in Sec. III I, where β_2 is analytically continued across $r > 0$, here when β_1 is analytically continued across $r < 0$, the Borel sum of the RSPT series switches branches and is discontinuous across the cut. A doubly-exponentially-small imaginary series appears that explicitly cancels the implicit discontinuity in the sum of the RSPT series. Unlike the semi-infinite β_2 case, there is here a new technical feature—the first index of the W Whittaker function is necessarily a power series in $(2r)^{-1}$. This feature leads to *logarithmic* terms in the expansion for $\Delta\beta_1^{\{2\}}$.

A. QSC wave function at $\xi = 0$

Near $\xi = 0$, Eq. (10) is Whittaker's equation [cf. Eq (33)],

$$[-(d/d\xi)^2+\tfrac{1}{4}r^2-r\beta_1/\xi+\tfrac{1}{4}(m^2-1)/\xi^2]\Phi_{[0]}\sim 0\ , \tag{128}$$

and the QSC wave function regular at the origin has the form

$$\Phi_{[0]}=\frac{1}{m!}(d\phi_{[0]}/d\xi)^{-1/2}M_{b_{[0]},m/2}(r\phi_{[0]})\ . \tag{129}$$

The function $\phi_{[0]}$, which plays the "action" role, depends on both ξ and r: $\phi_{[0]}=\phi_{[0]}(\xi,r)$. The boundary condition at $\xi=0$ is

$$\phi_{[0]}(0,r)=0\ . \tag{130}$$

$\phi_{[0]}$ satisfies the Riccati equation [cf. Eq. (35)],

$$-\left[\frac{d\phi_{[0]}}{d\xi}\right]^2\left[\frac{1}{4}-\frac{b_{[0]}}{r\phi_{[0]}}+\frac{m^2-1}{4r^2\phi_{[0]}^2}\right]-\frac{1}{r^2}\left[\frac{d\phi_{[0]}}{d\xi}\right]^{1/2}\frac{d^2}{d\xi^2}\left[\frac{d\phi_{[0]}}{d\xi}\right]^{-1/2}+\frac{1}{4}-\frac{\beta_1}{r\xi}-\frac{\beta_1+2\beta_2}{r(\xi+2)}+\frac{m^2-1}{r^2\xi^2(\xi+2)^2}=0\ . \tag{131}$$

Expanding β_1 and $\phi_{[0]}$ in powers of $(2r)^{-1}$ and solving recursively, one finds that

$$\phi_{[0]}=\sum_{N=0}^{\infty}\phi_{[0]}^{(N)}(\xi)(2r)^{-N}\ ,$$
$$\beta_1=\sum_{N=0}^{\infty}\beta_1^{(N)}(2r)^{-N}\ , \tag{132}$$

$$\phi_{[0]}^{(0)}=\xi\ , \tag{133}$$

$$\phi_{[0]}^{(1)}=-4(\beta_1^{(0)}+2\beta_2^{(0)})\ln(1+\tfrac{1}{2}\xi)\ , \tag{134}$$

$$\beta_1^{(0)}=b_{[0]}\ , \tag{135}$$

$$\beta_1^{(1)}=-2b_{[0]}(\beta_1^{(0)}+2\beta_2^{(0)})-\tfrac{1}{2}(m^2-1)\ , \tag{136}$$

and so forth. The value of $b_{[0]}$ is to be obtained by matching $\Phi_{[0]}$ with the QSC function that behaves correctly at ∞. The $\beta_1^{(N)}$ are determined so that the $\phi_{[0]}^{(N+1)}$ are analytic and zero at $\xi=0$, just as was the case for the $\beta_2^{(N)}$ in Sec. III B. The $\beta_1^{(N)}$ will turn out to be the RSPT coefficients.

B. QSC wave function at $\xi=-2$

Near $\xi=-2$, Eq. (10) is again a Whittaker equation,

$$[-(d/d\xi)^2+\tfrac{1}{4}r^2-r(\beta_1+2\beta_2)/(\xi+2)+\tfrac{1}{4}(m^2-1)/(\xi+2)^2]\Phi_{[0]}\sim 0\ . \tag{137}$$

The QSC wave function that is exponentially small as $r\xi\to+\infty$ (but singular at $\xi=-2$) is [cf. Eq. (115)]

$$\Phi_{[-2]}=(d\phi_{[-2]}/d\xi)^{-1/2}W_{b_{[-2]},m/2}(r\phi_{[-2]})\ , \tag{138}$$

with boundary condition

$$\phi_{[-2]}(-2,r)=0\ . \tag{139}$$

The Riccati equation for $\phi_{[-2]}$ is nominally the same as for $\phi_{[0]}$, Eq. (131), and is not repeated here. One solves for $\phi_{[-2]}$ as an expansion,

$$\phi_{[-2]}=\sum_{N=0}^{\infty}\phi_{[-2]}^{(N)}(\xi)(2r)^{-N}\ . \tag{140}$$

In contrast with the method of solution for $\phi_{[0]}$, however, both $\beta_1^{(N)}$ and $\beta_2^{(N)}$ are already fixed and cannot be adjusted to make $\phi_{[-2]}^{(N+1)}$ vanish at $\xi=-2$. Here that role is taken by the index $b_{[-2]}$ on the Whittaker W function. The index $b_{[-2]}$ is given by an expansion in $(2r)^{-1}$,

$$b_{[-2]}=\sum_{N=0}^{\infty}b_{[-2]}^{(N)}(2r)^{-N}\ . \tag{141}$$

One finds that

$$\phi_{[-2]}^{(0)}=\xi+2\ , \tag{142}$$

$$\phi_{[-2]}^{(1)}=-4\beta_1^{(0)}\ln(-\tfrac{1}{2}\xi)\ , \tag{143}$$

$$b_{[-2]}^{(0)}=\beta_1^{(0)}+2\beta_2^{(0)}\ , \tag{144}$$

$$b_{[-2]}^{(1)}=2(\beta_1^{(1)}+\beta_2^{(1)}) \tag{145}$$

$$=-4(\beta_1^{(0)}+\beta_2^{(0)})^2=-4n^2\ , \tag{146}$$

and so forth.

C. Determination of $b_{[0]}$ by matching $\Phi_{[0]}$ and $\Phi_{[-2]}$

The index $b_{[0]}$ is evaluated by the condition that the two QSC functions be the same. Two cases are considered: r large, but with small phase; and r large, but with phase more negative than $-\pi$. In the former case one gets RSPT, while in the latter there is in addition an imaginary second-exponential-order series.

The logic is by now familiar. When $r\phi_{[0]}$ and $r\phi_{[-2]}$, viz., $r\xi$ and $r(\xi+2)$, are large, the asymptotic expansions for the Whittaker functions give

$$\Phi_{[-2]}\sim r^{b_{[-2]}}(\xi+2)^{b_{[-2]}}(-\tfrac{1}{2}\xi)^{\beta_1^{(0)}}e^{-r(\xi+2)/2}\ , \tag{147}$$

$$\Phi_{[0]}\sim\frac{e^{\pm i\pi(m/2+1/2-b_{[0]})}}{\Gamma(\tfrac{1}{2}m+\tfrac{1}{2}+b_{[0]})}(r\xi)^{b_{[0]}}\times[(\xi+2)/2]^{\beta_1^{(0)}+2\beta_2^{(0)}}e^{-r\xi/2}+\frac{1}{\Gamma(\tfrac{1}{2}m+\tfrac{1}{2}-b_{[0]})}(r\xi)^{-b_{[0]}}\times[(\xi+2)/2]^{-\beta_1^{(0)}-2\beta_2^{(0)}}e^{+r\xi/2}\ . \tag{148}$$

[The $\pm$ corresponds to the sign of $\arg(r\phi_{[0]})$.] The elimination of the positive exponential $e^{+r\xi/2}$ series from $\Phi_{[0]}$ requires that $\tfrac{1}{2}m+\tfrac{1}{2}-b_{[0]}$ be zero or a negative integer.

$$b_{[0]}=n_1+\tfrac{1}{2}m+\tfrac{1}{2}\quad (n_1=0,1,2,\ldots)\ . \tag{149}$$

Thus $b_{[0]}$ is the unperturbed eigenvalue of Eq. (15). [Cf. also Eq. (17).]

To get at the cut in $\beta_1(r)$ on the negative r axis, we now consider the possibility that r becomes negative. It turns out that $b_{[0]}$ has a different expansion when $\arg r<-\pi$. Notice from Eq. (18) that the singularity at $u=-2r$, which originally occurs at an unphysical value of the physical variable u, moves into the physical domain when r is negative. Note also that to keep the physical variable u approximately positive as r is made negative, ξ will also have to be made negative, but in the opposite sense of r, since $u=r\xi$. Further, it will be convenient to match the two QSC Φ's in the region between their "anchor" points, $\xi=0$ and -2. Consequently the primary region of interest for ξ is near -1, and for $2+\xi$ near $+1$. The dominant term $r\xi$ in $r\phi_{[0]}$ will be large and stay approximately positive, while the dominant term $r(\xi+2)$ in $r\phi_{[2]}$ will become large and approximately negative. The negative z axis, however, is a branch cut for the Borel sum of the asymptotic series for $W_{b,m/2}(z)$. The asymptotic expansion for $W_{b,m/2}(z)$ above the negative z axis and its *analytic continuation* across the negative z axis will differ by an exponentially small expansion that cancels the discontinuity in the Borel sum.

To make this last point more precise, let $z=e^{-\pi i}z'$, and let z' be approximately real and positive. When $\arg z=-\pi-\epsilon$ ($\epsilon>0$), the standard asymptotic expansion for $W_{b,m/2}(z)$ is not applicable. The correct expansion may be obtained by first applying the circuital relation[20] (here $\arg z'=-\epsilon<0$),

$$W_{b,m/2}(z'e^{-\pi i})=e^{-2\pi ib}W_{b,m/2}(z'e^{\pi i})-2\pi i\frac{e^{-\pi ib}W_{-b,m/2}(z')}{\Gamma(\tfrac{1}{2}+\tfrac{1}{2}m-b)\Gamma(\tfrac{1}{2}-\tfrac{1}{2}m-b)}\ , \tag{150}$$

and then by using the asymptotic expansions for the standard domains. As a consequence, $\Phi_{[-2]}$ will now have a positive exponential series, and $b_{[0]}$ will be different from $n_1+\tfrac{1}{2}m+\tfrac{1}{2}$. Let

$$b_{[0]}=\beta_1^{(0)}+\Delta b_{[0]}\ . \tag{151}$$

Also define $\delta b_{[-2]}$ by

$$\delta b_{[-2]}=b_{[-2]}-b_{[-2]}^{(0)}=\sum_{N=1}^{\infty}b_{[-2]}^{(N)}(2r)^{-N}+O(\Delta b_{[0]})\ . \tag{152}$$

Note that Δ has been used exclusively to denote exponentially small quantities. In this case $\delta b_{[-2]}$ is not exponentially small, and δ has been used instead of Δ.

To determine $\Delta b_{[0]}$, one obtains the following matching equation, which is the analog of Eqs. (105) and (120), and which is a simple consequence of Eqs. (55), (58), and (150):

$$\pi^{-1}\sin(\pi\Delta b_{[0]})=\frac{2\pi i(-1)^m e^{+\pi i\Delta b_{[0]}}}{\Gamma(n_1+m+1+\Delta b_{[0]})\Gamma(n_1+1+\Delta b_{[0]})}$$
$$\times\pi^{-2}\sin^2(\pi\delta b_{[-2]})\Gamma(n_1+2n_2+2m+2+\delta b_{[-2]})\Gamma(n_1+2n_2+m+2+\delta b_{[-2]})$$
$$\times\frac{W_{\beta_1^{(0)}+\Delta b_{[0]},m/2}(r\phi_{(0)})}{e^{+\pi i(\beta_1^{(0)}+\Delta b_{[0]})}W_{-\beta_1^{(0)}-\Delta b_{[0]},m/2}(r\phi_{[0]}e^{+\pi i})}\ \frac{e^{-\pi ib_{[-2]}}W_{-b_{[-2]},m/2}(r\phi_{[-2]}e^{\pi i})}{e^{-2\pi ib_{[-2]}}W_{b_{[-2]},m/2}(r\phi_{[-2]}e^{2\pi i})}\quad (\mathrm{Im}r<-\pi)\ . \tag{153}$$

Since r is essentially negative, set $r=-r'$:

$$r'=e^{\pi i}r\quad (\arg r'=\epsilon<0)\ . \tag{154}$$

The right-hand side of Eq. (153) is $O(r'^k e^{-2r'})$ and is also to this order purely imaginary. Consequently we can write

$$\Delta b_{[0]}=i\Delta_i b_{[0]}^{(2)}+O(r'^k e^{-4r'})\ , \tag{155}$$

where

$$\Delta_i b_{[0]}^{(2)}=2\pi(-1)^m\frac{\sin^2(\pi\delta b_{[-2]})}{\pi^2}(2r')^{2\beta_1^{(0)}-2b_{[-2]}^{(0)}-2\delta b_{[-2]}}e^{-2r'}$$
$$\times\frac{\Gamma(n_1+2n_2+2m+2+\delta b_{[-2]})\Gamma(n_1+2n_2+m+2+\delta b_{[-2]})}{n_1!(n_1+m)!}$$
$$\times(\tfrac{1}{2}e^{-\pi i}\phi_{[0]})^{2\beta_1^{(0)}}(\tfrac{1}{2}\phi_{[-2]})^{-2b_{[-2]}}e^{r'(\phi_{[0]}-\phi_{[-2]}+2)}\frac{{}_2F_0(-n_1,-n_1-m;;+(r'\phi_{[0]})^{-1})}{{}_2F_0(n_1+m+1,n_1+1;;-(r'\phi_{[0]})^{-1})}$$
$$\times\frac{{}_2F_0(n_1+2n_2+m+2+\delta b_{[-2]},n_1+2n_2+2m+2+\delta b_{[-2]};;-(r'\phi_{[-2]})^{-1})}{{}_2F_0(-n_1-2n_2-m-1-\delta b_{[-2]},-n_1-2n_2-2m-1-\delta b_{[-2]};;+(r'\phi_{[-2]})^{-1})} \tag{156}$$

$$\sim 2\pi(-1)^m 16n^4 \frac{(n_1+2n_2+2m+1)!(n_1+2n_2+m+1)!}{n_1!(n_1+m)!}(2r')^{-4\beta_2^{(0)}-2}e^{-2r'}$$
$$\times\left[1-\frac{1}{2r'}\{8n^2\ln(2r')-4n^2+12(\beta_2^{(0)})^2-(m^2-1)-8n+12\beta_2^{(0)}\right.$$
$$\left.-4n^2[\psi(n_1+2n_2+m+2)+\psi(n_1+2n_2+2m+2)]\}+O[r'^{-2}(\ln r')^2]\right] . \tag{157}$$

The complete evaluation of Eq. (156) is somewhat more tedious than the preceding similar cases because of the necessity for expanding the $\delta b_{[-2]}$ series out from the two Γ functions, the $\sin^2$, the $(\frac{1}{2}\phi_{[-2]})^{-2b_{[-2]}}$, and the $(2r')^{\delta b_{[-2]}}$, the last of which leads to subseries proportional to powers of $(2r')^{-1}\ln(2r')$. It is possible to avoid expanding out the generalized hypergeometrics. Since the expression is really independent of ξ, it can be evaluated at a special value of ξ. If $\xi=\infty$, then the generalized hypergeometrics are evaluated at 0 where they are unity.

After evaluating $\Delta_i b\{{}^{2}_{0}\}$, the corresponding imaginary doubly-exponentially-small contribution to the discontinuity of β_1 on the negative axis can be obtained via

$$\Delta_i\beta_1^{\{2\}}=\Delta_i b\{{}^{2}_{0}\}\sum_{N=0}^{\infty}\frac{d\beta_1^{(N)}}{d\beta_1^{(0)}}(-2r')^{-N} . \tag{158}$$

As for the β_2 cases, there are also other methods that avoid derivatives of the RSPT series, but we shall not go into the details here.

V. EXPANSION FOR $E(R)$ FROM THE EXPANSIONS FOR $\beta_1(r)$ AND $\beta_2(r)$

A. Preliminaries

The asymptotic expansion for $E(R)$ in terms of $(2R)^{-1}$ can be obtained from Eq. (12) for E in terms of β_1 and β_2, from Eqs. (24) and (26) for the RSPT expansions, and from the various equations of Secs. III and IV for the exponentially small series contributing to β_1 and β_2, but only after r has been found explicitly as a function of R from the implicit Eq. (13), $R(r)=r[\beta_1(r)+\beta_2(r)]$. The process is mainly algebraic. The main complication is that the transformation itself from r to R contains exponentially small terms. The purpose of this section is to clarify the process and to sketch the necessary steps.

Note that β_1 and β_2 appear in E and $R(r)$ only as the sum $\beta_1+\beta_2$, which we denote by γ:

$$\gamma(r)=\beta_1(r)+\beta_2(r) , \tag{159}$$

$$\gamma^{(N)}=\beta_1^{(N)}+\beta_2^{(N)} , \tag{160}$$

$$\Delta\gamma^{\{q\}}=\Delta\beta_1^{\{q\}}+\Delta\beta_2^{\{q\}}\quad (q=1,2,\ldots) , \tag{161}$$

and so forth. Further, we denote by γ_0 the formal power series

$$\gamma_0(r)=\sum_{N=0}^{\infty}\gamma^{(N)}(2r)^{-N} . \tag{162}$$

In the expression of r as a function of R, there will be a power-series contribution that we denote by r_0, and that is the formal power-series solution of

$$\frac{1}{2r_0}=\frac{\gamma_0(r_0(R))}{2R} . \tag{163}$$

By means of Lagrange's formula,[19] the solution can in fact be immediately written:

$$\frac{1}{2r_0}=\frac{n}{2R}+\sum_{N=1}^{\infty}\left[\frac{n}{2R}\right]^{N+1}\sum_{\substack{i_1,i_2,\ldots,i_N\\(i_1+2i_2+\cdots+Ni_N=N)}}\frac{N!(\gamma^{(1)}/n)^{i_1}(\gamma^{(2)}/n)^{i_2}\cdots(\gamma^{(N)}/n)^{i_N}}{\left[N+1-\sum_k i_k\right]!i_1!i_2!\cdots i_N!} \tag{164}$$

$$=\frac{n}{2R}+\left[\frac{n}{2R}\right]^2\frac{\gamma^{(1)}}{n}+\left[\frac{n}{2R}\right]^3\left[\frac{\gamma^{(2)}}{n}+\frac{(\gamma^{(1)})^2}{n^2}\right]+\cdots . \tag{165}$$

Here n is the usual principal quantum number. Note that $\gamma^{(0)}=n$, $\gamma^{(1)}=-2n^2$, and that the "natural" expansion parameter is $n/2R$. In a similar fashion the RSPT expansion for $E(R)$ can be written

$$\sum_{N=0}^{\infty}E^{(N)}(2R/n)^{-N}=-\tfrac{1}{2}\gamma_0^{-2}(r_0) \tag{166}$$

$$=\frac{-1}{2n^2}+n^{-2}\sum_{N=1}^{\infty}\left[\frac{n}{2R}\right]^N\sum_{\substack{i_1,i_2,\ldots,i_N\\(i_1+2i_2+\cdots+Ni_N=N)}}\frac{(N-3)!(\gamma^{(1)}/n)^{i_1}(\gamma^{(2)}/n)^{i_2}\cdots(\gamma^{(N)}/n)^{i_N}}{\left[N-2-\sum_k i_k\right]!i_1!i_2!\cdots i_N!} \tag{167}$$

$$=\frac{-1}{2n^2}+\left[\frac{n}{2R}\right]\frac{\gamma^{(1)}}{n^3}+\left[\frac{n}{2R}\right]^2\left[\frac{\gamma^{(2)}}{n^3}-\frac{\frac{1}{2}(\gamma^{(1)})^2}{n^4}\right]+\cdots . \tag{168}$$

The aim now is to express the exponentially small series in E, namely $\Delta E^{\{1\}}$, $\Delta E^{\{2\}}$, etc., entirely in terms of $\gamma_0(r_0)$, $\Delta\gamma^{\{1\}}(r_0)$, $\Delta\gamma^{\{2\}}(r_0)$, etc. That is, the $\Delta E^{\{q\}}$ should be put into a form in which the exponentially small contributions Δr to $r=r_0+\Delta r$ are expanded out explicitly as a function of r_0, and the remaining r_0 dependence can be replaced by its power series in R, Eq. (164). In fact, by two successive expansions of $E=-\frac{1}{2}\gamma^{-2}$ [Eq. (12)], the first with respect to $\Delta\gamma$, the second with respect to $\Delta(r^{-1})$, one obtains

$$E=E_{\rm RSPT}+\Delta E=E_{\rm RSPT}+\Delta E^{\{1\}}+\Delta E^{\{2\}}+\cdots \tag{169}$$

$$=-\tfrac{1}{2}\gamma_0^{-2}(r)+\Delta\gamma(r)\gamma_0^{-3}(r)-\tfrac{3}{2}[\Delta\gamma(r)]^2\gamma_0^{-4}(r)+\cdots \tag{170}$$

$$=-\tfrac{1}{2}\gamma_0(r_0)^{-2}-\tfrac{1}{2}\Delta(r^{-1})[(d/dr_0^{-1})\gamma_0(r_0)^{-2}]-\tfrac{1}{4}[\Delta(r^{-1})]^2[(d/dr_0^{-1})^2\gamma_0(r_0)^{-2}]+\cdots$$
$$+\Delta\gamma_0(r_0)[\gamma_0(r_0)^{-3}]-\tfrac{3}{2}[\Delta\gamma_0(r_0)]^2[\gamma_0(r_0)^{-4}]+\cdots+\Delta(r^{-1})(d/dr_0^{-1})[\Delta\gamma(r_0)\gamma_0(r_0)^{-3}]+\cdots \; . \tag{171}$$

The $\Delta(r^{-1})$ can be expressed directly in terms of ΔE, Eq. (169); the ΔE can then be obtained recursively, as will be shown in the next several paragraphs:

$$r^{-1}=R^{-1}\gamma=R^{-1}(-2E)^{-1/2}=r_0^{-1}+\Delta(r^{-1}) \; , \tag{172}$$

$$\Delta(r^{-1})=R^{-1}\Delta E[(-2E_{\rm RSPT})^{-3/2}]$$
$$+\tfrac{3}{2}R^{-1}(\Delta E)^2[(-2E_{\rm RSPT})^{-5/2}]+\cdots \tag{173}$$
$$=\Delta E[r_0^{-1}\gamma_0(r_0)^2]$$
$$+\tfrac{3}{2}(\Delta E)^2[r_0^{-1}\gamma_0(r_0)^4]+\cdots \; , \tag{174}$$

where $E=E_{\rm RSPT}+\Delta E$ has been expanded around $E_{\rm RSPT}=-\frac{1}{2}\gamma_0(r_0)^{-2}$.

B. First exponential order

From Eqs. (171) and (174) the following preliminary formula for $\Delta E^{\{1\}}$ can be obtained:

$$\Delta E^{\{1\}}=\frac{\Delta\gamma^{\{1\}}(r_0)}{\gamma_0^3(r_0)-r_0^{-1}\gamma_0^2(r_0)(d/dr_0^{-1})\gamma_0(r_0)} \; . \tag{175}$$

The final formula for $\Delta E^{\{1\}}$ results from inserting Eq. (164) for r_0 into Eq. (175) and using the appropriate equations for $\Delta\gamma^{\{1\}}(r_0)$ developed in previous sections: Eqs. (64), (65), (69), (83), (126), (127), and (159)–(161). The first few terms are

$$\Delta E^{\{1\}}=\pm\frac{(2R/n)^{2\beta_2^{(0)}}e^{-R/n-n}}{n^3 n_2!(n_2+m)!}\times\left[1+\left[\frac{n}{2R}\right][2n\beta_1^{(0)}-4(\beta_2^{(0)})^2+\beta_2^{(1)}+2n^2]+O(R^{-2})\right] . \tag{176}$$

C. Imaginary second exponential order; more on the approximate formula of Brézin and Zinn-Justin

In exactly the same way that Eq. (175) was obtained, one gets for the imaginary second-exponential-order series, i.e., the imaginary part of $\Delta E^{\{2\}}$ when R is real and positive,

$$\Delta E^{\{2\}}=\Delta_r E^{\{2\}}+i\Delta_i E^{\{2\}} \; , \tag{177}$$

$$\Delta_i E^{\{2\}}=\frac{\Delta_i\gamma^{\{2\}}(r_0)}{\gamma_0^3(r_0)-r_0^{-1}\gamma_0^2(r_0)(d/dr_0^{-1})\gamma_0(r_0)} \; . \tag{178}$$

When the series (164) for r_0 is substituted into the denominator and into the appropriate expressions for $\Delta_i\gamma^{\{2\}}$, then one gets the desired formula for $\Delta_i(E)^{\{2\}}$. Up to two terms (but not to three) the formula is, except for sign, πn^3 times the square of $\Delta E^{\{1\}}$, Eq. (176):

$$\Delta_i E^{\{2\}}=\mp\pi n^3(\Delta E^{\{1\}})^2[1+O(R^{-2})] \quad (\pm{\rm Im}R\ge 0) \; . \tag{179}$$

Apart from the adjustment by the factor n^3, this result is the approximation of Brézin and Zinn-Justin,[12] demonstrated to be valid to only two terms for the ground state by Čížek, Clay, and Paldus[13] numerically, and by Damburg and Propin analytically.[14] In fact, it is not difficult to see that the exact relationship is

$$\mp\pi n^3\frac{\Delta_i E^{\{2\}}}{(\Delta E^{\{1\}})^2}=\frac{n^3(d/d\beta_2^{(0)})\gamma_0(r_0)}{\gamma_0(r_0)^3-r_0^{-1}\gamma_0(r_0)^2(d/dr_0^{-1})\gamma_0(r_0)} \tag{180}$$

$$=1-(2r_0)^{-2}4\beta_2^{(0)}n+O(r^{-3}) \tag{181}$$

$$=1-(2R/n)^{-2}4\beta_2^{(0)}n+O(R^{-3}) \; . \tag{182}$$

Thus, exactly two terms are given correctly by the gap-squared formula for *every* state.

D. Real second exponential order

The extraction of the real second-exponential-order series for $\Delta_r E^{\{2\}}$ is more tedious, as can be seen from the following equation obtained from Eqs. (171) and (174), and in which all quantities are to be evaluated at $r=r_0$, the power series given by Eq. (164):

$$\Delta_r E^{\{2\}} = \gamma_0^{-3}\Delta_r\gamma^{\{2\}} - \tfrac{3}{2}\gamma_0^{-4}(\Delta\gamma^{\{1\}})^2 + \gamma_0^{-1}\Delta_r E^{\{2\}} r_0^{-1}(d\gamma_0/dr_0^{-1}) + \Delta E^{\{1\}}[\gamma_0^{-1}r_0^{-1}(d\Delta\gamma^{\{1\}}/dr_0^{-1}) - 3\gamma_0^{-2}\Delta\gamma^{\{1\}}r_0^{-1}(d\gamma_0/dr_0^{-1})] + (\Delta E^{\{1\}})^2\{\tfrac{3}{2}r_0^{-1}(d\gamma_0/dr_0^{-1}) + \tfrac{1}{2}\gamma_0 r_0^{-2}[d^2\gamma_0/(dr_0^{-1})^2] - \tfrac{3}{2}r_0^{-2}(d\gamma_0/dr_0^{-1})^2\} . \tag{183}$$

The leading term comes from $\Delta E^{\{1\}}\gamma_0^{-1}r_0^{-1}(d\Delta\gamma^{\{1\}}/dr_0^{-1})$, since $r^{-1}(d/dr^{-1})e^{-r} = re^{-r}$. Consequently we obtain for the first few terms of $\Delta_r E^{\{2\}}$

$$\Delta_r E^{\{2\}} = \frac{\Delta E^{\{1\}}\Delta\gamma^{\{1\}}(r_0 - 2\beta_0^{(0)})}{\gamma_0 - r_0^{-1}(d\gamma_0/dr_0^{-1})}[1+O(r^{-2})] + \frac{\Delta_r\gamma^{(2)} - \tfrac{3}{2}\gamma_0^{-1}(\Delta\gamma^{\{1\}})^2}{\gamma_0^3 - \gamma_0^2 r_0^{-1}(d\gamma_0/dr_0^{-1})} \tag{184}$$

$$= R(\Delta E^{\{1\}})^2\gamma_0[1-(2r_0)^{-1}(3+2\beta_2^{(0)}) + O(r_0^{-2})] + n^{-3}\Delta_r b^{\{2\}}[1+O(r_0^{-2})] , \tag{185}$$

and finally,

$$\Delta_r(E)^{\{2\}} = nR(\Delta E^{\{1\}})^2\left[1 - \frac{n}{2R}[3+2\beta_2^{(0)} + 2n^2 + 2n\psi(n_2+1) + 2n\psi(n_2+m+1)] + \frac{n}{2R}[4n\ln(2R/n)] + O(R^{-2})\right] . \tag{186}$$

Note the term $(n/2R)\ln(2R/n)$.

E. Discontinuity in $E(R)$ for R negative

The last expression we obtain in this section is for the discontinuity of E across the negative R axis, namely, $E(e^{-\pi i}R') - E(e^{+\pi i}R')$, with $\arg R' = 0$. The contributing expressions are Eqs. (156)–(161), (171), and (174). By the same logic that led to Eqs. (175) and (178) for $\Delta E^{\{1\}}$ and $\Delta_i E^{\{2\}}$, one can see that with $r_0' = -r_0$,

$$E(e^{-\pi i}R') - E(e^{+\pi i}R') = \frac{i\Delta_i\beta_2^{\{2\}}}{\gamma_0^3(-r_0') - r_0'^{-1}\gamma_0^2(-r_0')(d/dr_0'^{-1})\gamma_0(-r_0')} \tag{187}$$

$$= in^{-3}\Delta_i b_{[0]}^{\{2\}}[1+O(r_0'^{-2})] \tag{188}$$

$$= 2\pi i(-1)^m 16n\frac{(n_1+2n_2+2m+1)!(n_1+2n_2+m+1)!}{n_1!(n_1+m)!}(2R'/n)^{-4\beta_2^{(0)}-2}e^{-2R'/n+2n} \times \left[1 - \frac{n}{2R'}[8n^2\ln(2R'/n) + 12(\beta_2^{(0)})^2 - (m^2-1) - 8\beta_1^{(0)} + 4\beta_2^{(0)} - 4n^2[\psi(n_1+2n_2+2m+2) + \psi(n_1+2n_2+m+2)] - 12n\beta_1^{(0)} - 4n - 8n\beta_2^{(0)}] + O[R'^{-2}(\ln R')^2]\right] . \tag{189}$$

Again, notice the term $(n/2R')\ln(2R'/n)$.

VI. DISPERSION RELATIONS AND ASYMPTOTICS OF THE RSPT COEFFICIENTS

Dispersion relations are pertinent to the large-N behavior of the RSPT coefficients, whose asymptotic behavior they permit to be expressed as moments of the discontinuity of the imaginary part of the eigenvalue across the real axis. Dispersion relations arise from Cauchy's integral formula by enlargement of the contour to wrap around a branch cut. (These are standard arguments. See, e.g., Simon.[23])

Consider first the β_2 RSPT series, whose Borel sum is $\beta_1'(re^{-i\pi})$ for $\mathrm{Im}\, r \geq 0$ (see Sec. III I). One is led to the formula (see Sec. IV of Ref. 6 for a rigorous discussion)

$$\beta_1'(re^{-\pi i}) = \frac{1}{2\pi i}\int_0^\infty \frac{\beta_1'(re^{-\pi i}) - \beta_1'(re^{+\pi i})}{z-r}dz , \tag{190}$$

where again, this integral is meant only in the sense of power-series expansion. The discontinuity in β_1' is given by Eq. (124), which is ∓ 2 times the imaginary series entering the expansion for β_2 when $\pm\mathrm{Im}\, r \geq 0$. This fact, along with the expansion of the denominator $(z-r)$ in a geometric series, gives [cf. Eq. (100)]

$$\beta_2^{(N)} \sim -\int_0^\infty (2z)^{N-1}\Delta b^{\{1\}}(z)^2 q(z)d(2z) \tag{191}$$

$$\sim \pi^{-1}\int_0^{\infty+i\epsilon}(2z)^{N-1}\Delta_i\beta_2^{\{2\}}(z)d(2z) \quad (\epsilon > 0) \tag{192}$$

$$\sim -\frac{(N+4n_2+2m+1)!}{(n_2!)^2[(n_2+m)!]^2} \times \left[1 - \frac{12(\beta_2^{(0)})^2 + 4\beta_2^{(0)} - m^2 + 1}{N+4n_2+2m+1} + O(N^{-2})\right] . \tag{193}$$

In this way the discontinuity in $\beta_1'(re^{-\pi i})$, which is imaginary and of second exponential order, determines the asymptotics of the RSPT $\beta_2^{(N)}$.

Similar considerations apply to the RSPT series for β_1, which is Borel summable to the eigenvalue of the modified Eq. (15) when $\beta_1'(re^{-\pi i})$ is used for β_2. (See again Ref. 6 for the rigorous details.) Since, however, $\beta_1(r)$ also has a cut for negative r, as well as the cut for positive r induced by the cut in $\beta_1'(re^{-\pi i})$, there are two terms in the dispersion relation:

$$\beta_1(r)=\frac{1}{2\pi i}\int_0^\infty \frac{\beta_1(z)-\beta_1(ze^{2\pi i})}{z-r}dz+\frac{1}{2\pi i}\int_{\infty e^{\pi i}}^0 \frac{-\beta_1(ze^{-2\pi i})+\beta_1(z)}{z-r}dz \tag{194}$$

$$=\frac{1}{2\pi i}\int_0^\infty \frac{\beta_1(z)-\beta_1(ze^{2\pi i})}{z-r}dz+\frac{1}{2\pi i}\int_0^\infty \frac{\beta_1(z'e^{-\pi i})-\beta_1(z'e^{+\pi i})}{z'+r}dz' \, . \tag{195}$$

As for the β_1' (i.e., β_2) dispersion relation, the discontinuity on the positive axis, $\beta_1(z)-\beta_1(ze^{2\pi i})$, is imaginary and of second exponential order: it is $\mp 2i$ times the $(\Delta_i\beta_1^{\{2\}})_{\rm ind}$ of Eqs. (126) and (127). The discontinuity on the negative axis is given by Eqs. (156)–(158). Just as for $\beta_2^{(N)}$, one obtains for $\beta_1^{(N)}$

$$\beta_1^{(N)}\sim\pi^{-1}\int_0^{\infty+i\epsilon}(2z)^{N-1}[\Delta_i\beta_1^{\{2\}}(z)]_{\rm ind}d(2z)+(2\pi)^{-1}\int_0^\infty(-2z')^{N-1}\Delta_i\beta_1^{\{2\}}(z')d(2z') \quad (\epsilon>0) \tag{196}$$

$$\sim\frac{(N+4n_2+2m)!}{(n_2!)^2[(n_2+m)!]^2}\left[4\beta_1^{(0)}-\frac{48\beta_1^{(0)}(\beta_2^{(0)})^2+12(\beta_1^{(0)})^2-(1+4\beta_1^{(0)})(m^2-1)}{N+4n_2+2m}+O(N^{-2})\right]$$
$$+(-1)^{m+N-1}16n^4\frac{(n_1+2n_2+2m+1)!(n_1+2n_2+m+1)!}{n_1!(n_1+m)!}(N-4n_2-2m-5)!$$
$$\times\left[1+\frac{4n^2-12(\beta_2^{(0)})^2+m^2-1+12n-12\beta_2^{(0)}}{N-4n_2-2m-5}\right.$$
$$\left.-\frac{4n^2[2\psi(N-4n_2-2m-5)-\psi(n_1+2n_2+2m+2)-\psi(n_1+2n_2+m+2)]}{N-4n_2-2m-5}+O[N^{-2}(\ln N^2)]\right] . \tag{197}$$

Note that the dominant asymptotic behavior coming from the positive cut is a same-sign $(N+4n_2+2m)!$, but that buried a factor of N^{5+8n_2+4m} down is an alternating-sign contribution that also involves a $\ln N$ dependence, since $\psi(N)\sim\ln N+O(N^{-1})$. Because of its relative smallness, the alternating-sign contribution is not immediately apparent from a numerical table of the $\beta_1^{(N)}$, but careful numerical analysis can detect it.

Similar considerations apply to the RSPT series for $E(R)$, which is Borel summable[5,6] to $-\frac{1}{2}[\beta_1'(r_0e^{-i\pi})+\beta_1(r_0,\beta_1'(r_0e^{-\pi i}))]^{-2}$. That is, instead of the *real* β_2 of Eq. (11), one puts into both Eqs. (10) and (12) the analytic continuation of the β_1' of Eqs. (113) and (114). There are two cuts in this Borel sum, with the key second-exponential-order quantities given by Eqs. (172), (173), and (182). The resulting asymptotics for the $E^{(N)}$ are

$$E^{(N)}\sim\pi^{-1}\int_0^{\infty+i\epsilon}(2z/n)^{N-1}\Delta_iE^{\{2\}}(z)d(2z/n)$$
$$+(2\pi i)^{-1}\int_0^\infty(2z'/n)^{N-1}[E(R'e^{-\pi i})-E(R'e^{+\pi i})]d(2z'/n) \tag{198}$$

$$\sim-\frac{e^{-2n}}{n^3(n_2!)^2[(n_2+m)!]^2}(N+4n_2+2m+1)!\left[1+\frac{4n\beta_1^{(0)}-8(\beta_2^{(0)})^2+2\beta_2^{(1)}+4n^2}{N+4n_2+2m+1}+O(N^{-2})\right]$$
$$+(-1)^{m+N-1}e^{2n}16n^4\frac{(n_1+2n_2+2m+1)!(n_1+2n_2+m+1)!}{n^3n_1!(n_1+m)!}(N-4n_2-2m-5)!$$
$$\times\left[1+\frac{12n^2-12(\beta_2^{(0)})^2+m^2-1+12n-12\beta_2^{(0)}-4n\beta_2^{(0)}}{N-4n_2-2m-5}\right.$$
$$\left.-\frac{4n^2[2\psi(N-4n_2-2m-5)-\psi(n_1+2n_2+2m+2)-\psi(n_1+2n_2+m+2)]}{N-4n_2-2m-5}+O(N^{-2}(\ln N)^2)\right] . \tag{199}$$

Again, note the alternating-sign contribution that is down by a factor of N^{6+8n_2+4m} from the dominant same-sign $(N+4n_2+2m+1)!$ behavior. The alternating-sign contribution is not readily apparent from a table of the $E^{(N)}$, but careful numerical analysis can detect it. In fact, it was this unsuspected alternating-sign contribution that was responsible for the prior difficulty in carrying out the Bender-Wu analysis of the numerical $E^{(N)}$ for the ground state.[13] This point will be discussed in more detail in Secs. IX and X.

VII. JWKB-LIKE FORMULATION

The purpose of this section is to simplify the practical procedure for calculating the $O(e^{-r})$ and imaginary $O(e^{-2r})$ expansions for β_1 and β_2. The procedure so far involves three steps: (i) solution of a Riccati equation for ϕ, e.g., Eq. (35); (ii) determination of the index shift, e.g., $\Delta b^{\{1\}}$ of Eq. (64); (iii) determination of the ratio $q(r)$ by, e.g., Eq. (69) or (83). What complicates the procedure is the presence of ϕ^{-1} and ϕ^{-2} in the Riccati equation, which is the consequence of starting from the Whittaker confluent hypergeometric function. The alternative is to start from an exponential function—i.e., the JWKB-like form—which leads to a much simpler Riccati equation, but which then requires a "connection formula" and an alternative method to calculate $q(r)$.

The JWKB-like form for the QSC wave function Φ_2 [cf. Eqs. (31) and (32)] is

$$\Phi_2=(dS/d\eta)^{-1/2}(Ae^{-rS/2}+Be^{+rS/2}) , \qquad (200)$$

where $S=S(\eta,r)$ satisfies the Riccati equation,

$$\frac{1}{4}\left[\frac{dS}{d\eta}\right]^2=\frac{1}{4}-\frac{\beta_2}{4}\left[\frac{1}{\eta}+\frac{1}{2-\eta}\right] +\frac{m^2-1}{4r^2}\left[\frac{1}{\eta}+\frac{1}{2-\eta}\right]^2 -\frac{1}{r^2}\left[\frac{dS}{d\eta}\right]^{1/2}\frac{d^2}{d\eta^2}\left[\frac{dS}{d\eta}\right]^{-1/2} . \qquad (201)$$

We assume for $S(\eta,r)$ an expansion of the form

$$S(\eta,r)\sim\sum_{N=0}^{\infty}S^{(N)}(\eta)(2r)^{-N}+O(r^ke^{-r}) , \qquad (202)$$

where in fact the $S^{(N)}(\eta)$ can be obtained directly from the QSC wave function by using the asymptotic expansion (56) for the Whittaker function and then rearranging terms appropriately. For instance, Eqs. (200) and (61) imply that

$$A(dS/d\eta)^{-1/2}e^{-rS/2} =\frac{(-1)^{n_2}(2r)^{\beta_2^{(0)}}}{(n_2+m)!} \times\eta^{\beta_2^{(0)}}(2-\eta)^{-\beta_2^{(0)}}e^{-r\eta/2}[1+O(r^{-1})] . \qquad (203)$$

Then,

$$S=c+\eta+(2r)^{-1}4\beta_2^{(0)}\ln\left[\frac{2-\eta}{\eta}\right]+O(r^{-2}) , \qquad (204)$$

$$A=(-1)^{n_2}e^{+rc/2}(2r)^{2\beta_2^{(0)}}/(n_2+m)! , \qquad (205)$$

where c is a constant (with respect to η) related to the normalization (see below).

The main point, however, is not to obtain the $S^{(N)}$ from the $\phi^{(N)}$, but figuratively the reverse, because the $S^{(N)}$ are much easier to obtain directly from Eq. (201) than the $\phi^{(N)}$ from Eq. (35). For instance, given already that $dS^{(0)}/d\eta=1$, then for $N\geq 1$, $S^{(N)}$ satisfies

$$dS^{(N)}/d\eta=-\tfrac{1}{2}\sum_{k=1}^{N-1}(dS^{(k)}/d\eta)(dS^{(N-k)}/d\eta)-4\beta_2^{(N-1)}[\eta^{-1}+(2-\eta)^{-1}] +2\delta_{N,2}(m^2-1)[\eta^{-1}+(2-\eta)^{-1}]^2-8[(dS/d\eta)^{1/2}(d^2/d\eta^2)(dS/d\eta)^{-1/2}]^{(N-2)} , \qquad (206)$$

from which it follows that (see also immediately below)

$$dS^{(1)}/d\eta=-4\beta_2^{(0)}[\eta^{-1}+(2-\eta)^{-1}] , \qquad (207)$$

$$S^{(1)}=+4\beta_2^{(0)}\ln\left[\frac{2-\eta}{\eta}\right] , \qquad (208)$$

$$dS^{(2)}/d\eta=-8(\beta_2^{(0)})^2[\eta^{-1}+(2-\eta)^{-1}]^2 -4\beta_2^{(1)}[\eta^{-1}+(2-\eta)^{-1}] +2(m^2-1)[\eta^{-1}+(2-\eta)^{-1}]^2 \qquad (209)$$

$$\beta_2^{(1)}=-2(\beta_2^{(0)})^2+\tfrac{1}{2}(m^2-1) , \qquad (210)$$

$$S^{(2)}=-4\beta_2^{(1)}[\eta^{-1}-(2-\eta)^{-1}] , \qquad (211)$$

and so forth. There are two tricky points. The first is that the Riccati equation (201) involves only derivatives of S, and not S itself. The integration constants implicit in Eqs. (208) and (211) are therefore not determined by the Riccati equation; they will be explained in the next paragraph. The second point is that, apart from $S^{(1)}$, the $S^{(N)}$ for $N\geq 2$ cannot have a $\ln\eta$ dependence. That is, $\beta_2^{(N-1)}$ has the value that eliminates the η^{-1} term from the recursive Eq. (206) for $S^{(N)}$. A most important practical consequence turns out to be that for $N\geq 2$, $dS^{(N)}/d\eta$ is a polynomial $P_N(\eta^{-1})$ in η^{-1} of degree N, with no constant or first-order term, plus a similar polynomial in $(2-\eta)^{-1}$. Moreover, because of the symmetry of Eqs. (201) and (206) with respect to $\eta\rightarrow 2-\eta$, it follows that

$$dS^{(N)}/d\eta=P_N(\eta^{-1})+P_N[(2-\eta)^{-1}] . \qquad (212)$$

Thus, the $S^{(N)}$ for $N\geq 2$ have a much simpler structure than the $\phi^{(N)}$ in that they are polynomials requiring only $N-1$ coefficients, and they have no complicated logarithmic terms.

Now we return to the integration-constant problem, which affects both the absolute normalization, which cannot be determined from the differential equation anyway, and the relative weights of the $e^{\pm rS/2}$ components, which is a connection-formula problem solved here easily because the overall Schrödinger equation is symmetric under $\eta\rightarrow 2-\eta$. The solution is to make $S^{(N)}$ satisfy

$$S^{(N)}(2-\eta)=S^{(N)}(\eta) , \qquad (213)$$

and to take A/B in Eq. (200) to be ± 1. This then fixes also $S^{(0)}$,

$$S^{(0)}=\eta-1\ , \tag{214}$$

as well as the integration constants for all $S^{(N)}$.

However, there are still two major remaining problems: how to get $\Delta\beta_2^{\{1\}}$ and $\Delta_i\beta_2^{\{2\}}$ from Φ_2 in JWKB form. In Sec. III the procedure depended first on calculating the Whittaker index shift, which does not occur here, and second, the ratio $q(r)$. Here we can obtain $\Delta\beta_2^{\{1\}}$ from the two functions $\Phi_2^{(\pm)}$,

$$\Phi_2^{(\pm)}=(dS/d\eta)^{-1/2}(e^{-rS/2}\pm e^{+rS/2})\ , \tag{215}$$

via the standard current density formula, Eq. (79), which here becomes

$$2\Delta\beta_2^{\{1\}}=-2\Big/\int_0^{\eta}(dS/d\eta)^{-1}(e^{-rS}-e^{rS})\times[\eta^{-1}+(2-\eta)^{-1}]d\eta\quad(0\ll\eta\ll2)\ . \tag{216}$$

By the same argument as in Sec. III E, Eq. (216) can be put in the form

$$\Delta\beta_2^{\{1\}}=-e^{-r}\Big/\int_0^{\infty}(dS/d\eta)^{-1}e^{-r(S+1)}\times[\eta^{-1}+(2-\eta)^{-1}]d\eta\ , \tag{217}$$

where the integral in Eq. (217) is meant only in the sense of a series in $(2r)^{-1}$, obtained by appropriate expansion of the integrand, followed by integration term by term.

The determination of the imaginary second-exponential-order series $\Delta_i\beta_2^{\{2\}}$ could also be obtained from the JWKB function by a current-density formula, if one had the requisite connection formula. Unfortunately, we have not found a way to get the right formula without going directly through the Whittaker function. However, we can get $\Delta_i\beta_2^{\{2\}}$ via Eq. (101) from the square of $\Delta\beta_2^{\{1\}}$ and from $q(r)$, the latter of which can be solved for directly in the JWKB approach. Note that $q(r)=d\beta_{2,\text{RSPT}}/d\beta_2^{(0)}$ is a series in $(2r)^{-1}$ [Eq. (69)]. Let

$$T^{(N)}(\eta)\equiv dS^{(N)}(\eta)/d\beta_2^{(0)}\ . \tag{218}$$

Then T and $q(r)$ satisfy an equation obtained by differentiating the Riccati equation (201) with respect to $\beta_2^{(0)}$:

$$\frac{1}{2}\frac{dS}{d\eta}\frac{dT}{d\eta}=-r^{-1}q(r)\left[\frac{1}{\eta}+\frac{1}{2-\eta}\right]-r^{-2}\frac{1}{2}\frac{dT}{d\eta}\left[\frac{dS}{d\eta}\right]^{-1/2}\frac{d^2}{d\eta^2}\left[\frac{dS}{d\eta}\right]^{-1/2}+r^{-2}\frac{1}{2}\left[\frac{dS}{d\eta}\right]^{-1/2}\frac{d^2}{d\eta^2}\left[\frac{dS}{d\eta}\right]^{-3/2}\frac{dT}{d\eta}\ . \tag{219}$$

Further, by taking the $\beta_2^{(0)}$ derivative of the recursive Eq. (206), one obtains

$$dT^{(N)}/d\eta=-\sum_{k=0}^{N-1}(dT^{(k)}/d\eta)(dS^{(N-k)}/d\eta)-4q^{(N-1)}[\eta^{-1}+(2-\eta)^{-1}]-4[(dT/d\eta)(dS/d\eta)^{-1/2}(d^2/d\eta^2)(dS/d\eta)^{-1/2}-(dS/d\eta)^{1/2}(d^2/d\eta^2)(dS/d\eta)^{-3/2}(dT/d\eta)]^{(N-2)}\ . \tag{220}$$

One then finds (recall that $q^{(0)}=1$) that

$$T^{(0)}=0\ , \tag{221}$$

$$dT^{(1)}/d\eta=-4[\eta^{-1}(2-\eta)^{-1}]\ , \tag{222}$$

$$T^{(1)}=+4\ln\left[\frac{2-\eta}{\eta}\right]\ , \tag{223}$$

$$dT^{(2)}/d\eta=-16\beta_2^{(0)}[\eta^{-1}+(2-\eta)^{-1}]^2-4q^{(1)}[\eta^{-1}+(2-\eta)^{-1}]\ , \tag{224}$$

$$q^{(1)}=-4\beta_2^{(0)}\ , \tag{225}$$

$$T^{(2)}=16\beta_2^{(0)}[\eta^{-1}-(2-\eta)^{-1}]\ , \tag{226}$$

and so forth. As is by now a familiar argument, the value of $q^{(N-1)}$ is obtained by eliminating the η^{-1} term in the equation [Eq. (220)] for $dT^{(N)}/d\eta$ for $N\geq2$. In such a way $q(r)$ can be obtained, and consequently $\Delta_i\beta_2^{\{2\}}$ via Eq. (101).

Finally, we consider the two contributions to β_1: $(\Delta\beta_1^{\{1\}}+i\Delta_i\beta_1^{\{2\}})_{\text{ind}}$ and $i\Delta_i\beta_1^{\{2\}}(-r)$ (the discontinuity at negative r). The induced terms are needed to high order. They can be calculated from Eq. (127) with the RSPT wave function, and thus require no further comment. The discontinuity for negative r, on the other hand, will not be taken further than the few orders given here explicitly, and so the JWKB approach will not be sketched.

This now completes the theoretical discussion of the computation of the asymptotic expansions for β_1, β_2, and E. In the remaining sections we give numerical illustrations of the various terms in the expansions, their asymptotics, and their interrelations.

VIII. NUMERICAL CHARACTERIZATION OF THE β_2 SERIES

In this section we tabulate and discuss the asymptotics for the various series contributing to the asymptotic expansion of β_2. First we list in Tables I—III the terms of the RSPT series, the exponentially small gap series $\Delta\beta_2^{\{1\}}$, and the doubly-exponentially-small imaginary series $\Delta_i\beta_2^{\{2\}}$, all through fifty-first order in $(2r)^{-1}$, for the ground state (for which $n_2=0$ and $m=0$) and for two excited states for which n_2 and m are (1,0) and (0,1). We

TABLE I. Coefficients for the RSPT series, the $\Delta\beta_2^{\{1\}}$ series, and the $\Delta_i\beta_2^{\{2\}}$ series, as defined by Eqs. (26), (227), and (228) of the text, for the ($n_2=0, m=0$) ground state of β_2.

Order N	$\beta_2^{(N)}$	Coefficient $c^{\{1\}(N)}$	$c^{\{2\}(N)}$
0	5.00000 00000 00000 00000 00000 000 x 10^{-1}	1.00000 00000 00000 00000 00000 000 x 10^{0}	1.00000 00000 00000 00000 00000 000 x 10^{0}
1	-1.00000 00000 00000 00000 00000 000 x 10^{0}	-4.00000 00000 00000 00000 00000 000 x 10^{0}	-6.00000 00000 00000 00000 00000 000 x 10^{0}
2	-1.00000 00000 00000 00000 00000 000 x 10^{0}	-3.00000 00000 00000 00000 00000 000 x 10^{0}	2.00000 00000 00000 00000 00000 000 x 10^{0}
3	-4.00000 00000 00000 00000 00000 000 x 10^{0}	-2.00000 00000 00000 00000 00000 000 x 10^{1}	-1.60000 00000 00000 00000 00000 000 x 10^{1}
4	-2.30000 00000 00000 00000 00000 000 x 10^{1}	-1.46000 00000 00000 00000 00000 000 x 10^{2}	-1.31000 00000 00000 00000 00000 000 x 10^{2}
5	-1.64000 00000 00000 00000 00000 000 x 10^{2}	-1.24000 00000 00000 00000 00000 000 x 10^{3}	-1.18600 00000 00000 00000 00000 000 x 10^{3}
6	-1.36200 00000 00000 00000 00000 000 x 10^{3}	-1.18390 00000 00000 00000 00000 000 x 10^{4}	-1.18100 00000 00000 00000 00000 000 x 10^{4}
7	-1.27440 00000 00000 00000 00000 000 x 10^{4}	-1.24324 00000 00000 00000 00000 000 x 10^{5}	-1.27960 00000 00000 00000 00000 000 x 10^{5}
8	-1.31707 00000 00000 00000 00000 000 x 10^{5}	-1.41649 00000 00000 00000 00000 000 x 10^{6}	-1.49465 40000 00000 00000 00000 000 x 10^{6}
9	-1.48424 40000 00000 00000 00000 000 x 10^{6}	-1.73543 12000 00000 00000 00000 000 x 10^{7}	-1.86934 68000 00000 00000 00000 000 x 10^{7}
10	-1.80783 02000 00000 00000 00000 000 x 10^{7}	-2.27232 04200 00000 00000 00000 000 x 10^{8}	-2.49095 24400 00000 00000 00000 000 x 10^{8}
11	-2.36476 47200 00000 00000 00000 000 x 10^{8}	-3.16578 38160 00000 00000 00000 000 x 10^{9}	-3.52338 30400 00000 00000 00000 000 x 10^{9}
12	-3.30587 16700 00000 00000 00000 000 x 10^{9}	-4.67728 16692 00000 00000 00000 000 x 10^{10}	-5.27508 14163 00000 00000 00000 000 x 10^{10}
13	-4.92007 90504 00000 00000 00000 000 x 10^{10}	-7.30893 64286 40000 00000 00000 000 x 10^{11}	-8.33998 05415 40000 00000 00000 000 x 10^{11}
14	-7.77049 28925 20000 00000 00000 000 x 10^{11}	-1.20530 61361 62700 00000 00000 000 x 10^{13}	-1.38965 93049 57800 00000 00000 000 x 10^{13}
15	-1.29869 09942 92800 00000 00000 000 x 10^{13}	-2.09349 93948 78760 00000 00000 000 x 10^{14}	-2.43608 16100 60240 00000 00000 000 x 10^{14}
16	-2.29119 96110 22270 00000 00000 000 x 10^{14}	-3.82297 63917 58058 00000 00000 000 x 10^{15}	-4.48542 46645 03802 00000 00000 000 x 10^{15}
17	-4.25726 70215 18900 00000 00000 000 x 10^{15}	-7.32739 10035 20413 60000 00000 000 x 10^{16}	-8.66093 78935 33990 80000 00000 000 x 10^{16}
18	-8.31362 93369 26679 00000 00000 000 x 10^{16}	-1.47167 45118 75833 30200 00000 000 x 10^{18}	-1.75113 16654 27886 86800 00000 000 x 10^{18}
19	-1.70286 51859 52650 20000 00000 000 x 10^{18}	-3.09248 48922 41491 97040 00000 000 x 10^{19}	-3.70189 81237 24444 08640 00000 000 x 10^{19}
20	-3.65163 71245 95240 29140 00000 000 x 10^{19}	-6.78854 08446 99841 64988 00000 000 x 10^{20}	-8.17064 74365 64111 78302 00000 000 x 10^{20}
21	-8.18363 62546 55226 91640 00000 000 x 10^{20}	-1.55445 81687 12466 66800 80000 000 x 10^{22}	-1.88020 75120 84454 55611 40000 000 x 10^{22}
22	-1.91352 06010 34558 15834 84000 000 x 10^{22}	-3.70764 85296 68338 29993 46200 000 x 10^{23}	-4.50486 43609 14752 88996 53200 000 x 10^{23}
23	-4.66085 99868 46674 53748 97600 000 x 10^{23}	-9.19903 08925 25069 64112 14480 000 x 10^{24}	-1.12231 29845 29462 33492 30384 000 x 10^{25}
24	-1.18087 09875 31777 21528 18974 000 x 10^{25}	-2.37105 59152 59105 74586 84410 000 x 10^{26}	-2.90371 73545 26023 57510 80214 000 x 10^{26}
25	-3.10768 72059 67308 72311 17543 200 x 10^{26}	-6.34097 00820 77188 20855 34988 320 x 10^{27}	-7.79251 53228 08283 84083 62822 960 x 10^{27}
26	-8.48401 03159 03761 99466 43713 720 x 10^{27}	-1.75738 83051 43272 09774 64771 848 x 10^{29}	-2.16661 87672 77887 09157 84670 735 x 10^{29}
27	-2.39970 72843 52675 68333 74424 069 x 10^{29}	-5.04182 10457 38398 35811 33937 983 x 10^{30}	-6.23434 80127 14026 00283 15075 752 x 10^{30}
28	-7.02431 79168 22741 72523 31191 884 x 10^{30}	-1.49571 64288 09167 61657 52989 120 x 10^{32}	-1.85459 34956 33853 10071 88516 430 x 10^{32}
29	-2.12551 33457 46545 09323 16169 555 x 10^{32}	-4.58365 26145 22014 91608 59148 195 x 10^{33}	-5.69801 46494 80673 26407 95454 135 x 10^{33}
30	-6.64185 83025 05175 43644 14212 211 x 10^{33}	-1.44962 62146 16932 19240 75245 053 x 10^{35}	-1.80636 35257 23279 36841 49310 267 x 10^{35}
31	-2.14120 94328 88922 08476 96351 560 x 10^{35}	-4.72699 60495 98641 44352 22329 589 x 10^{36}	-5.90342 08831 68021 20850 61900 585 x 10^{36}
32	-7.11497 97941 70213 53743 47647 260 x 10^{36}	-1.58789 82879 84635 97550 95887 989 x 10^{38}	-1.98723 43570 83596 13745 71503 926 x 10^{38}
33	-2.43476 01998 75947 84045 16985 059 x 10^{38}	-5.49048 73994 89535 01901 11200 699 x 10^{39}	-6.88476 83858 90553 46760 93238 203 x 10^{39}
34	-8.57333 80341 53255 41652 72258 532 x 10^{39}	-1.95258 70796 48423 03941 78559 903 x 10^{41}	-2.45295 71861 49525 55312 40654 798 x 10^{41}
35	-3.10396 56319 28989 55910 55864 809 x 10^{41}	-7.13671 83784 92300 82039 52528 491 x 10^{42}	-8.98116 61087 52749 84174 69544 320 x 10^{42}
36	-1.15461 29420 60619 29018 30718 129 x 10^{43}	-2.67897 35693 68627 74424 09797 058 x 10^{44}	-3.37687 21026 81779 45823 79481 983 x 10^{44}
37	-4.40964 88093 35437 27416 23730 083 x 10^{44}	-1.03211 43799 72823 92389 66487 791 x 10^{46}	-1.30300 74990 96156 42092 56503 281 x 10^{46}
38	-1.72794 59793 86441 83558 55102 283 x 10^{46}	-4.07848 00503 49129 07760 85440 066 x 10^{47}	-5.15649 19022 80787 89237 58353 474 x 10^{47}
39	-6.94287 54341 60981 32809 73866 808 x 10^{47}	-1.65201 67304 14025 34334 48890 893 x 10^{49}	-2.09157 84455 26994 94656 43290 908 x 10^{49}
40	-2.85870 36167 95211 42358 58706 384 x 10^{49}	-6.85524 00386 77524 26835 40750 117 x 10^{50}	-8.69071 33574 32356 42848 37178 851 x 10^{50}
41	-1.20550 51343 76258 72332 02260 750 x 10^{51}	-2.91260 01443 40255 49058 66339 557 x 10^{52}	-3.69707 50313 60110 25599 19234 567 x 10^{52}
42	-5.20355 49106 85414 14568 64618 160 x 10^{52}	-1.26636 09070 46195 03421 76231 613 x 10^{54}	-1.60935 99125 18770 97479 16088 058 x 10^{54}
43	-2.29791 48686 18532 42916 00762 910 x 10^{54}	-5.63158 90714 31873 69861 52625 228 x 10^{55}	-7.16506 99757 94250 99220 85582 926 x 10^{55}
44	-1.03765 25193 10435 21015 42299 284 x 10^{56}	-2.56028 91040 18442 42650 46072 008 x 10^{57}	-3.26099 00973 70612 52788 02117 622 x 10^{57}
45	-4.78900 15564 75344 94313 70950 205 x 10^{57}	-1.18940 07060 37608 89247 32088 544 x 10^{59}	-1.51648 59630 26241 83995 46170 311 x 10^{59}
46	-2.25794 09433 59019 65094 16354 837 x 10^{59}	-5.64356 23561 95807 13378 84812 863 x 10^{60}	-7.20266 80972 58068 07728 82973 260 x 10^{60}
47	-1.08708 24854 82559 41046 75467 189 x 10^{61}	-2.73386 47676 07054 08529 73618 875 x 10^{62}	-3.49243 55429 46068 17903 53647 809 x 10^{62}
48	-5.34207 78495 67110 04754 84898 385 x 10^{62}	-1.35150 99684 21553 94756 34420 727 x 10^{64}	-1.72808 26951 32021 67269 69868 230 x 10^{64}
49	-2.67841 86985 57226 31974 80156 238 x 10^{64}	-6.81564 40356 14582 87447 90262 544 x 10^{65}	-8.72227 43608 43794 99073 75183 599 x 10^{65}
50	-1.36960 98468 21709 74345 22170 539 x 10^{66}	-3.50488 21329 08820 26687 38878 986 x 10^{67}	-4.48909 20002 24446 57754 83776 332 x 10^{67}
51	-7.14005 39439 56397 53456 22192 581 x 10^{67}	-1.83720 85116 61938 24749 17709 789 x 10^{69}	-2.35500 24637 87773 35815 26898 324 x 10^{69}

use the notation $c^{\{1\}(N)}$ and $c^{\{2\}(N)}$ for the series coefficients for the two exponentially small quantities [cf. also Eqs. (54) and (99)]:

$$\Delta\beta_2^{\{1\}} = \pm \frac{(2r)^{2\beta_2^{(0)}} e^{-r}}{n_2!(n_2+m)!} \sum_{N=0}^{\infty} c^{\{1\}(N)} (2r)^{-N} , \qquad (227)$$

$$\Delta_i\beta_2^{\{2\}} = \mp\pi \frac{(2r)^{4\beta_2^{(0)}} e^{-2r}}{[n_2!(n_2+m)!]^2} \times \sum_{N=0}^{\infty} c^{\{2\}(N)} (2r)^{-N} \quad (\pm \mathrm{Im}\, r \geq 0) . \qquad (228)$$

Notice that the coefficients (at least those with fewer than the maximum number of significant digits) appear to be

TABLE II. Coefficients for the RSPT series, the $\Delta\beta_2^{\{1\}}$ series, and the $\Delta_i\beta_2^{\{2\}}$ series, as defined by Eqs. (26), (227), and (228) of the text, for the ($n_2=1, m=0$) excited state of β_2.

Order		Coefficient	
N	$\beta_2^{(N)}$	$c^{(1)(N)}$	$c^{(2)(N)}$
0	1.50000 00000 00000 00000 00000 000 x 10^{0}	1.00000 00000 00000 00000 00000 0 x 10^{0}	1.00000 00000 00000 00000 00000 0 x 10^{0}
1	-5.00000 00000 00000 00000 00000 000 x 10^{0}	-2.00000 00000 00000 00000 00000 0 x 10^{1}	-3.40000 00000 00000 00000 00000 0 x 10^{1}
2	-1.50000 00000 00000 00000 00000 000 x 10^{1}	7.90000 00000 00000 00000 00000 0 x 10^{1}	3.82000 00000 00000 00000 00000 0 x 10^{2}
3	-1.24000 00000 00000 00000 00000 000 x 10^{2}	-1.40000 00000 00000 00000 00000 0 x 10^{2}	-1.80000 00000 00000 00000 00000 0 x 10^{3}
4	-1.40100 00000 00000 00000 00000 000 x 10^{3}	-1.44900 00000 00000 00000 00000 0 x 10^{3}	2.75900 00000 00000 00000 00000 0 x 10^{3}
5	-1.89080 00000 00000 00000 00000 000 x 10^{4}	-2.71800 00000 00000 00000 00000 0 x 10^{4}	-1.28420 00000 00000 00000 00000 0 x 10^{4}
6	-2.87790 00000 00000 00000 00000 000 x 10^{5}	-5.29102 00000 00000 00000 00000 0 x 10^{5}	-2.29554 00000 00000 00000 00000 0 x 10^{5}
7	-4.79032 80000 00000 00000 00000 000 x 10^{6}	-1.07178 00000 00000 00000 00000 0 x 10^{7}	-5.00120 00000 00000 00000 00000 0 x 10^{6}
8	-8.55929 01000 00000 00000 00000 000 x 10^{7}	-2.25598 17700 00000 00000 00000 0 x 10^{8}	-1.11861 67700 00000 00000 00000 0 x 10^{8}
9	-1.62192 49080 00000 00000 00000 000 x 10^{9}	-4.92147 11960 00000 00000 00000 0 x 10^{9}	-2.57053 15820 00000 00000 00000 0 x 10^{9}
10	-3.23250 68706 00000 00000 00000 000 x 10^{10}	-1.10988 94357 40000 00000 00000 0 x 10^{11}	-6.06569 00350 00000 00000 00000 0 x 10^{10}
11	-6.73608 46023 20000 00000 00000 000 x 10^{11}	-2.58205 23355 44000 00000 00000 0 x 10^{12}	-1.46892 76000 40000 00000 00000 0 x 10^{12}
12	-1.46142 79030 98600 00000 00000 000 x 10^{13}	-6.18612 91921 55800 00000 00000 0 x 10^{13}	-3.64875 11428 09800 00000 00000 0 x 10^{13}
13	-3.29060 69379 17680 00000 00000 000 x 10^{14}	-1.52432 98050 56760 00000 00000 0 x 10^{15}	-9.29198 45888 50280 00000 00000 0 x 10^{14}
14	-7.67143 36414 01820 00000 00000 000 x 10^{15}	-3.85941 36242 03950 00000 00000 0 x 10^{16}	-2.42511 91536 09848 40000 00000 0 x 10^{16}
15	-1.84843 79970 80646 24000 00000 000 x 10^{17}	-1.00330 60726 60789 13600 00000 0 x 10^{18}	-6.48485 69907 24364 80000 00000 0 x 10^{17}
16	-4.59699 61209 97360 74900 00000 000 x 10^{18}	-2.67663 65632 22320 18290 00000 0 x 10^{19}	-1.77635 67105 06533 32930 00000 0 x 10^{19}
17	-1.17879 08355 26013 11180 00000 000 x 10^{20}	-7.32537 77992 96708 57596 00000 0 x 10^{20}	-4.98393 90973 42652 50038 00000 0 x 10^{20}
18	-3.11421 63901 20289 86921 00000 000 x 10^{21}	-2.05610 83355 15227 58653 66000 0 x 10^{22}	-1.43219 30202 07219 22611 42000 0 x 10^{22}
19	-8.47114 92481 05832 81940 88000 000 x 10^{22}	-5.91784 77055 13196 97774 55200 0 x 10^{23}	-4.21508 26751 34774 24225 84800 0 x 10^{23}
20	-2.37139 51306 64353 18768 28460 000 x 10^{24}	-1.74636 02638 88521 58796 86698 0 x 10^{25}	-1.27053 00054 98321 50863 56998 0 x 10^{25}
21	-6.82900 54018 38489 37056 42440 000 x 10^{25}	-5.28348 72967 01142 31949 67652 0 x 10^{26}	-3.92228 94820 09263 65812 74534 0 x 10^{26}
22	-2.02232 39028 84232 49825 83059 240 x 10^{27}	-1.63868 19398 02560 95274 51599 7 x 10^{28}	-1.24013 69787 85037 54869 30185 5 x 10^{28}
23	-6.15665 56058 51913 21565 96472 080 x 10^{28}	-5.20985 42615 91068 09353 90167 0 x 10^{29}	-4.01576 13158 67891 81492 67074 6 x 10^{29}
24	-1.92622 25172 07042 01876 03172 196 x 10^{30}	-1.69776 42417 31158 08294 82577 0 x 10^{31}	-1.33173 39805 98400 16783 83876 6 x 10^{31}
25	-6.19158 27043 12407 71637 60630 245 x 10^{31}	-5.67028 20309 90721 47662 47606 1 x 10^{32}	-4.52261 32888 36149 44369 21485 5 x 10^{32}
26	-2.04405 42323 48321 89800 46461 406 x 10^{33}	-1.94066 31196 26219 37173 29205 7 x 10^{34}	-1.57268 35502 19543 78418 88854 0 x 10^{34}
27	-6.92841 54288 88016 64480 78189 018 x 10^{34}	-6.80524 07901 98263 84893 67740 8 x 10^{35}	-5.59907 95879 18291 13573 03960 2 x 10^{35}
28	-2.41031 48241 35442 14985 99921 841 x 10^{36}	-2.44456 11469 58322 27853 54574 2 x 10^{37}	-2.04053 92869 53159 10947 16949 2 x 10^{37}
29	-8.60303 70969 35033 61034 45996 990 x 10^{37}	-8.99343 52514 02760 98447 98358 7 x 10^{38}	-7.61101 86968 89220 24321 04967 5 x 10^{38}
30	-3.14920 34143 86974 19796 00692 752 x 10^{39}	-3.38773 08077 53251 59474 22324 9 x 10^{40}	-2.90478 93346 26683 11651 43846 8 x 10^{40}
31	-1.18180 88928 18561 80957 86905 142 x 10^{41}	-1.30626 55389 85574 10499 99715 9 x 10^{42}	-1.13410 82383 50151 69426 32699 2 x 10^{42}
32	-4.54478 68051 15425 64706 98675 558 x 10^{42}	-5.15424 58570 19095 02936 34729 7 x 10^{43}	-4.52842 75237 74185 49325 41237 6 x 10^{43}
33	-1.79026 95612 40790 23279 03640 787 x 10^{44}	-2.08053 21720 25534 63296 61777 0 x 10^{45}	-1.84871 98441 10222 11599 98361 1 x 10^{45}
34	-7.22069 78673 35164 79148 63644 151 x 10^{45}	-8.58852 10932 50696 42439 84301 2 x 10^{46}	-7.71431 74222 19582 71894 45968 7 x 10^{46}
35	-2.98066 04197 44885 29279 22693 454 x 10^{47}	-3.62453 24148 46241 86913 83649 4 x 10^{48}	-3.28923 03154 46304 15004 74978 2 x 10^{48}
36	-1.25873 95363 48933 92704 37018 582 x 10^{49}	-1.56324 71918 70763 86589 89602 0 x 10^{50}	-1.43260 38556 26793 60235 53027 7 x 10^{50}
37	-5.43586 22112 53563 50247 58601 235 x 10^{50}	-6.88805 25148 76714 26733 14015 2 x 10^{51}	-6.37170 76617 73232 33429 33518 5 x 10^{51}
38	-2.39956 11218 76005 14118 81227 428 x 10^{52}	-3.09962 46018 18145 40738 35073 6 x 10^{53}	-2.89298 01806 22921 36021 74676 4 x 10^{53}
39	-1.08230 75925 96434 51732 05279 466 x 10^{54}	-1.42402 25909 58260 78956 41689 7 x 10^{55}	-1.34046 94982 60535 48097 75340 5 x 10^{55}
40	-4.98601 23372 61673 79697 98421 501 x 10^{55}	-6.67686 03852 12598 42070 65582 9 x 10^{56}	-6.33655 04597 44654 11445 74583 0 x 10^{56}
41	-2.34515 66937 30906 89225 10321 332 x 10^{57}	-3.19396 11943 63196 89651 27737 1 x 10^{58}	-3.05490 11323 29236 55442 10253 5 x 10^{58}
42	-1.12575 13315 75148 07995 20637 080 x 10^{59}	-1.55827 96259 78061 30025 50082 9 x 10^{60}	-1.50160 31266 46630 39406 28205 1 x 10^{60}
43	-5.51322 35319 95889 34088 37293 762 x 10^{60}	-7.75137 20404 41128 23447 33637 7 x 10^{61}	-7.52305 62992 97730 94890 80388 6 x 10^{61}
44	-2.75363 26072 06983 29451 35466 885 x 10^{62}	-3.92998 57306 41202 55583 30987 1 x 10^{63}	-3.84046 85805 09093 46782 66425 9 x 10^{63}
45	-1.40214 42335 29008 28314 25014 531 x 10^{64}	-2.03023 93933 85626 80333 32386 9 x 10^{65}	-1.99708 65621 87354 15592 29038 2 x 10^{65}
46	-7.27644 06986 88205 51053 60561 273 x 10^{65}	-1.06835 38389 14209 33412 91094 4 x 10^{67}	-1.05756 45263 27929 37460 55075 4 x 10^{67}
47	-3.84717 93139 33494 80978 96448 920 x 10^{67}	-5.72486 63011 85086 61970 23238 2 x 10^{68}	-5.70152 90109 74236 32455 17242 9 x 10^{68}
48	-2.07168 93981 50953 44764 69212 890 x 10^{69}	-3.12299 89365 32400 27393 64589 9 x 10^{70}	-3.12845 65088 91508 89186 25437 9 x 10^{70}
49	-1.13587 70317 33535 64658 77546 574 x 10^{71}	-1.73385 01676 79170 84494 86717 2 x 10^{72}	-1.74664 95254 45916 75763 02557 9 x 10^{72}
50	-6.33916 49503 26059 31915 32049 022 x 10^{72}	-9.79410 14748 54531 37172 30127 7 x 10^{73}	-9.91981 41758 09251 08270 34313 5 x 10^{73}
51	-3.59998 13761 20306 92394 57989 742 x 10^{74}	-5.62748 11044 41740 67063 02348 3 x 10^{75}	-5.72942 93811 75222 29516 04585 1 x 10^{75}

integers. The coefficients are estimated to be accurate to the precision reported, with uncertainty only in the last digit. Notice that for the ($n_2=1$, $m=0$) state, only 27 digits have been reported for the coefficients $c^{\{1\}(N)}$ and $c^{\{2\}(N)}$, two fewer than the 29 reported for the (0,0) and (0,1) states. The numerical error seems to depend on n_2.

It is interesting to examine numerically the prediction of the asymptotics of the $\beta_2^{(N)}$ by the dispersion relation [Eqs. (192) and (193)], which in the more general notation of Eq. (228) becomes

TABLE III. Coefficients for the RSPT series, the $\Delta\beta_2^{\{1\}}$ series, and the $\Delta_i\beta_2^{\{2\}}$ series, as defined by Eqs. (26), (227), and (228) of the text, for the $(n_2=0, m=1)$ excited state of β_2.

Order N	$\beta_2^{(N)}$	Coefficient $c^{(1)(N)}$	$c^{(2)(N)}$
0	1.00000 00000 00000 00000 00000 000 $\times 10^{0}$	1.00000 00000 00000 00000 00000 000 $\times 10^{0}$	1.00000 00000 00000 00000 00000 000 $\times 10^{0}$
1	-2.00000 00000 00000 00000 00000 000 $\times 10^{0}$	-1.00000 00000 00000 00000 00000 000 $\times 10^{1}$	-1.60000 00000 00000 00000 00000 000 $\times 10^{1}$
2	-4.00000 00000 00000 00000 00000 000 $\times 10^{0}$	8.00000 00000 00000 00000 00000 000 $\times 10^{0}$	6.40000 00000 00000 00000 00000 000 $\times 10^{1}$
3	-2.40000 00000 00000 00000 00000 000 $\times 10^{1}$	-4.80000 00000 00000 00000 00000 000 $\times 10^{1}$	-1.04000 00000 00000 00000 00000 000 $\times 10^{2}$
4	-2.00000 00000 00000 00000 00000 000 $\times 10^{2}$	-5.80000 00000 00000 00000 00000 000 $\times 10^{2}$	-3.28000 00000 00000 00000 00000 000 $\times 10^{2}$
5	-2.01600 00000 00000 00000 00000 000 $\times 10^{3}$	-7.48000 00000 00000 00000 00000 000 $\times 10^{3}$	-4.89600 00000 00000 00000 00000 000 $\times 10^{3}$
6	-2.31680 00000 00000 00000 00000 000 $\times 10^{4}$	-1.03568 00000 00000 00000 00000 000 $\times 10^{5}$	-7.28000 00000 00000 00000 00000 000 $\times 10^{4}$
7	-2.94144 00000 00000 00000 00000 000 $\times 10^{5}$	-1.52982 40000 00000 00000 00000 000 $\times 10^{6}$	-1.13612 80000 00000 00000 00000 000 $\times 10^{6}$
8	-4.04886 40000 00000 00000 00000 000 $\times 10^{6}$	-2.39283 52000 00000 00000 00000 000 $\times 10^{7}$	-1.85722 08000 00000 00000 00000 000 $\times 10^{7}$
9	-5.96958 72000 00000 00000 00000 000 $\times 10^{7}$	-3.93987 26400 00000 00000 00000 000 $\times 10^{8}$	-3.17245 05600 00000 00000 00000 000 $\times 10^{8}$
10	-9.35031 68000 00000 00000 00000 000 $\times 10^{8}$	-6.79920 53760 00000 00000 00000 000 $\times 10^{9}$	-5.65015 25760 00000 00000 00000 000 $\times 10^{9}$
11	-1.54693 27872 00000 00000 00000 000 $\times 10^{10}$	-1.22590 79884 80000 00000 00000 000 $\times 10^{11}$	-1.04728 20364 80000 00000 00000 000 $\times 10^{11}$
12	-2.69193 68371 20000 00000 00000 000 $\times 10^{11}$	-2.30392 03428 48000 00000 00000 000 $\times 10^{12}$	-2.01732 33895 68000 00000 00000 000 $\times 10^{12}$
13	-4.91201 56016 64000 00000 00000 000 $\times 10^{12}$	-4.50543 56797 82400 00000 00000 000 $\times 10^{13}$	-4.03372 18125 31200 00000 00000 000 $\times 10^{13}$
14	-9.37628 90723 32800 00000 00000 000 $\times 10^{13}$	-9.15592 81229 49120 00000 00000 000 $\times 10^{14}$	-8.36514 33929 06240 00000 00000 000 $\times 10^{14}$
15	-1.86885 76969 72800 00000 00000 000 $\times 10^{15}$	-1.93165 90899 22713 60000 00000 000 $\times 10^{16}$	-1.79793 93963 46265 60000 00000 000 $\times 10^{16}$
16	-3.88370 71338 67776 00000 00000 000 $\times 10^{16}$	-4.22741 50482 92408 32000 00000 000 $\times 10^{17}$	-4.00277 77477 65836 80000 00000 000 $\times 10^{17}$
17	-8.40420 68016 11857 92000 00000 000 $\times 10^{17}$	-9.59058 84493 80975 61600 00000 000 $\times 10^{18}$	-9.22605 31364 71498 75200 00000 000 $\times 10^{18}$
18	-1.89169 34886 99642 06080 00000 000 $\times 10^{19}$	-2.25415 45617 81600 41984 00000 000 $\times 10^{20}$	-2.20058 58918 34310 32832 00000 000 $\times 10^{20}$
19	-4.42462 17665 65281 05472 00000 000 $\times 10^{20}$	-5.48589 88501 96950 28633 60000 000 $\times 10^{21}$	-5.42916 44313 67332 99097 60000 000 $\times 10^{21}$
20	-1.07440 27756 35857 90894 08000 000 $\times 10^{22}$	-1.38165 27991 83060 69919 74400 000 $\times 10^{23}$	-1.38484 30328 17282 12963 32800 000 $\times 10^{23}$
21	-2.70603 51042 39472 98078 72000 000 $\times 10^{23}$	-3.59910 63521 10533 96414 05440 000 $\times 10^{24}$	-3.65033 35474 65427 44333 51680 000 $\times 10^{24}$
22	-7.06307 14522 84627 41507 27680 000 $\times 10^{24}$	-9.69136 19662 67827 05149 13280 000 $\times 10^{25}$	-9.93822 69721 12706 01209 77408 000 $\times 10^{25}$
23	-1.90884 86356 42899 25508 43187 200 $\times 10^{26}$	-2.69593 63553 29941 41437 42935 040 $\times 10^{27}$	-2.79316 96996 86573 81493 15215 360 $\times 10^{27}$
24	-5.33697 33102 89601 45846 41454 080 $\times 10^{27}$	-7.74284 03651 30866 09938 41119 232 $\times 10^{28}$	-8.09942 37604 10702 89308 06788 096 $\times 10^{28}$
25	-1.54239 78463 51307 58563 66488 781 $\times 10^{29}$	-2.29445 91630 54104 45539 96369 592 $\times 10^{30}$	-2.42173 23352 81385 51231 37515 684 $\times 10^{30}$
26	-4.60376 41702 78633 69811 98374 830 $\times 10^{30}$	-7.01080 26281 52372 76772 64822 010 $\times 10^{31}$	-7.46196 25743 21848 53308 91739 333 $\times 10^{31}$
27	-1.41804 17250 31727 51726 10206 309 $\times 10^{32}$	-2.20738 20760 34027 12384 02811 521 $\times 10^{33}$	-2.36793 61646 67898 62205 86112 125 $\times 10^{33}$
28	-4.50376 94527 22540 95973 68211 057 $\times 10^{33}$	-7.15688 43088 83317 05264 56626 571 $\times 10^{34}$	-7.73410 17795 78155 86706 42297 178 $\times 10^{34}$
29	-1.47378 96971 25289 26058 30488 482 $\times 10^{35}$	-2.38793 83703 43630 94475 80447 367 $\times 10^{36}$	-2.59839 90084 55357 53263 72962 166 $\times 10^{36}$
30	-4.96521 64280 81112 14342 78197 278 $\times 10^{36}$	-8.19396 72317 89302 91911 53902 723 $\times 10^{37}$	-8.97414 37133 40939 98093 29841 256 $\times 10^{37}$
31	-1.72094 08950 60214 53338 85764 683 $\times 10^{38}$	-2.88975 91120 63477 48480 58175 925 $\times 10^{39}$	-3.18427 23534 76594 72900 43246 414 $\times 10^{39}$
32	-6.13213 57385 70984 69034 47651 078 $\times 10^{39}$	-1.04678 09528 80914 92932 97202 597 $\times 10^{41}$	-1.16011 50478 78334 12209 56993 577 $\times 10^{41}$
33	-2.24481 12406 67547 79391 73805 946 $\times 10^{41}$	-3.89237 01919 74876 38441 55236 998 $\times 10^{42}$	-4.33725 58059 49575 09867 31546 774 $\times 10^{42}$
34	-8.43695 38955 83334 49409 59536 439 $\times 10^{42}$	-1.48484 64984 86378 34637 92912 871 $\times 10^{44}$	-1.66306 04740 10825 20485 42504 234 $\times 10^{44}$
35	-3.25353 84079 78630 75435 72353 408 $\times 10^{44}$	-5.80778 97647 62745 32334 30782 664 $\times 10^{45}$	-6.53646 37574 53146 48975 82917 538 $\times 10^{45}$
36	-1.28655 42403 03024 99411 24527 804 $\times 10^{46}$	-2.32789 27592 21978 16503 46432 946 $\times 10^{47}$	-2.63202 12722 45744 07511 67507 533 $\times 10^{47}$
37	-5.21374 94182 38823 50424 48239 120 $\times 10^{47}$	-9.55667 27556 83867 27111 41257 767 $\times 10^{48}$	-1.08523 75211 94378 82744 48132 443 $\times 10^{49}$
38	-2.16411 43365 49032 40103 03211 461 $\times 10^{49}$	-4.01623 40577 77871 93899 63445 474 $\times 10^{50}$	-4.57966 23345 86010 24148 98973 144 $\times 10^{50}$
39	-9.19572 63165 28012 99435 46621 835 $\times 10^{50}$	-1.72696 91957 80488 63154 53603 438 $\times 10^{52}$	-1.97700 10865 55540 07562 14630 475 $\times 10^{52}$
40	-3.99801 76984 58478 85839 30951 055 $\times 10^{52}$	-7.59444 06896 89895 50199 92081 660 $\times 10^{53}$	-8.72657 27525 64503 71852 92694 954 $\times 10^{53}$
41	-1.77763 30030 03953 13985 68352 041 $\times 10^{54}$	-3.41391 23547 10593 61242 09256 098 $\times 10^{55}$	-3.93685 37661 65573 34821 77509 223 $\times 10^{55}$
42	-8.07927 68518 20944 86792 92822 731 $\times 10^{55}$	-1.56805 46075 39565 68345 33212 958 $\times 10^{57}$	-1.81441 09847 33018 58730 45585 351 $\times 10^{57}$
43	-3.75178 66114 84874 93484 01114 947 $\times 10^{57}$	-7.35590 27477 51297 52543 24836 487 $\times 10^{58}$	-8.53928 15714 53621 25202 39539 069 $\times 10^{58}$
44	-1.77929 87191 74216 90990 68731 144 $\times 10^{59}$	-3.52287 37604 07422 17599 86641 306 $\times 10^{60}$	-4.10233 33480 91543 39763 79749 593 $\times 10^{60}$
45	-8.61433 48316 18318 76745 01538 475 $\times 10^{60}$	-1.72175 41174 38477 02490 31508 341 $\times 10^{62}$	-2.01092 15330 98022 79251 37733 026 $\times 10^{62}$
46	-4.25579 46361 88988 40652 73769 831 $\times 10^{62}$	-8.58402 18479 14235 85944 99103 971 $\times 10^{63}$	-1.00542 62179 42892 23922 90764 418 $\times 10^{64}$
47	-2.14464 78468 75634 72822 33920 275 $\times 10^{64}$	-4.36409 90995 97032 46814 62895 880 $\times 10^{65}$	-5.12552 10656 74151 60586 05945 406 $\times 10^{65}$
48	-1.10200 68188 84216 01455 22633 754 $\times 10^{66}$	-2.26165 57416 42607 33286 94221 006 $\times 10^{67}$	-2.66321 15861 13510 19355 32483 192 $\times 10^{67}$
49	-5.77175 57651 61523 65614 94220 444 $\times 10^{67}$	-1.19436 14723 88742 88435 17899 028 $\times 10^{69}$	-1.40995 51338 22096 70891 46864 535 $\times 10^{69}$
50	-3.08017 19432 47631 67846 14925 771 $\times 10^{69}$	-6.42505 42174 78515 31986 50090 213 $\times 10^{70}$	-7.60315 52960 37439 96066 53109 700 $\times 10^{70}$
51	-1.67432 05275 14734 41042 82490 310 $\times 10^{71}$	-3.51972 46750 67149 81233 74327 203 $\times 10^{72}$	-4.17477 40581 97506 34985 77375 030 $\times 10^{72}$

$$\beta_2^{(N)} \sim -\frac{(N+4n_2+2m+1)!}{(n_2!)^2[(n_2+m)!]^2} \times \left[1+\frac{c^{\{2\}(1)}}{N+4n_2+2m+1} + \frac{c^{\{2\}(2)}}{(N+4n_2+2m+1)(N+4n_2+2m)}+\cdots\right]. \quad (229)$$

In Table IV, the fit between the numerical and asymptotic $\beta_2^{(N)}$'s is displayed for the same three states for orders 10–150 (by tens). The agreement is similar to that for the RSPT of the one-dimensional anharmonic oscillator:[24] for large N it is impressive.

The expansion (229) has some of the character of an asymptotic expansion in that at first the partial sums approach the exact result, but then as the number of terms increases the partial sums eventually diverge. The partial

TABLE IV. Accuracy of the asymptotic formula for $\beta_2^{(N)}$ to k terms,

$$\beta_2^{(N)} \sim -\frac{(N+4n_2+2m+1)!}{(n_2!)^2[(n_2+m)!]^2}\left[1+\frac{c^{\{2\}(1)}}{N+4n_2+2m+1}+\frac{c^{\{2\}(2)}}{(N+4n_2+2m+1)(N+4n_2+2m)}+\cdots+\frac{c^{\{2\}(k)}}{(N+4n_2+2m+1)\cdots(N+4n_2+2m+2-k)}\right].$$

N	$-\beta_2^{(N)}$(exact)[a]	$-\beta_2^{(N)}$(asympt. to $k=k_{best}$)[b]	k_{best}[c]	k_{min}[d]	Number of significant figures[e] in sum to k terms for k = 0	5	10	15	20	25	30	35	40	45	50
	Ground state: n_2=0, m=0														
10	1.80783 02000 00000 00000 00000 000 x 10^{7}	1.81440 00000 00000 00000 00000 000 x 10^{7}	1	3	0	[1]	0								
20	3.65163 71245 95240 29140 00000 000 x 10^{19}	3.65181 12451 23148 80000 00000 000 x 10^{19}	9	9	0	3	[3]	2							
30	6.64185 83025 05175 43644 14212 211 x 10^{33}	6.64185 67341 40119 51127 36164 741 x 10^{33}	15	14	0	4	5	[6]	5	3					
40	2.85870 36167 95211 42358 58706 384 x 10^{49}	2.85870 36165 32667 95487 87068 898 x 10^{49}	20	19	0	5	7	8	[10]	7	6	3			
50	1.36960 98468 21709 74345 22170 539 x 10^{66}	1.36960 98468 21937 64957 80688 076 x 10^{66}	25	25	0	5	8	10	10	[12]	10	9	7	4	
60	4.57887 70826 33415 42505 00263 865 x 10^{83}	4.57887 70826 33417 88966 08031 516 x 10^{83}	30	30	1	6	9	11	13	13	[15]	13	12	10	8
70	7.78904 18221 69343 93085 42809 826 x 10^{101}	7.78904 18221 69343 93882 49608 962 x 10^{101}	35	35	1	6	10	12	14	15	16	[18]	16	15	14
80	5.36929 57277 99859 95287 33544 732 x 10^{120}	5.36929 57277 99859 95288 20414 138 x 10^{120}	40	40	1	7	11	14	16	17	18	19	[20]	19	18
90	1.26315 59649 87504 79228 93873 012 x 10^{140}	1.26315 59649 87504 79228 93902 279 x 10^{140}	45	45	1	7	11	14	17	19	21	21	22	[23]	22
100	8.86769 22459 42392 25888 59953 573 x 10^{159}	8.86769 22459 42392 25888 59953 849 x 10^{159}	50	50	1	7	12	15	18	21	22	24	24	25	[26]
110	1.66792 36392 98188 02740 52859 789 x 10^{180}	1.66792 36392 98188 02740 52859 790 x 10^{180}	51	51	1	8	12	16	.19	22	24	25	27	27	28
120	7.69396 26739 89238 59456 36348 094 x 10^{200}	7.69396 26739 89238 59456 36348 094 x 10^{200}	51	51	1	8	13	17	20	23	25	27	29	30	30
130	8.08449 83108 04571 30079 40173 389 x 10^{221}	8.08449 83108 04571 30079 40173 390 x 10^{221}	51	51	1	8	13	17	21	24	27	29	30	30	30
140	1.81755 22266 85751 87903 37981 498 x 10^{243}	1.81755 22266 85751 87903 37981 498 x 10^{243}	51	51	1	8	13	18	22	25	28	30	30	30	30
150	8.28512 52078 66554 03910 47333 007 x 10^{264}	8.28512 52078 66554 03910 47333 008 x 10^{264}	51	51	1	8	14	18	22	26	29	30	30	30	30
	Excited state: n_2=1, m=0														
10	3.23250 68706 00000 00000 00000 000 x 10^{10}	-2.97380 16000 00000 00000 00000 000 x 10^{10}	4	5	0	[1]	0								
20	2.37139 51306 64353 18768 28460 000 x 10^{24}	2.37795 00505 17954 23232 00000 000 x 10^{24}	5	6	0	[3]	1	0							
30	3.14920 34143 86974 19796 00692 752 x 10^{39}	3.14930 03360 49735 04774 14300 210 x 10^{39}	12	11	0	3	[3]	3	2	0					
40	4.98601 23372 61673 79697 98421 501 x 10^{55}	4.98601 72147 12094 77815 03028 937 x 10^{55}	18	17	0	3	4	5	[5]	4	3	0			
50	6.33916 49503 26059 31915 32049 022 x 10^{72}	6.33916 49515 77497 21832 82665 459 x 10^{72}	24	23	0	4	6	6	7	[8]	6	5	3	1	
60	4.63544 74996 34303 41334 53058 537 x 10^{90}	4.63544 74997 58604 50158 08091 176 x 10^{90}	29	28	0	5	7	8	9	9	[10]	9	8	6	4
70	1.51618 27058 20331 02030 62578 832 x 10^{109}	1.51618 27058 20245 49131 12712 302 x 10^{109}	35	34	0	5	7	9	10	11	12	[13]	12	11	9
80	1.83257 28247 25136 20913 17734 045 x 10^{128}	1.83257 28247 25136 11398 45455 552 x 10^{128}	40	39	0	5	8	10	12	13	14	14	[16]	14	13
90	7.05278 04064 63979 98969 48126 581 x 10^{147}	7.05278 04064 63979 98983 94935 738 x 10^{147}	45	44	0	6	9	11	13	15	16	17	17	[19]	17
100	7.67353 19779 42229 28064 17139 983 x 10^{167}	7.67353 19779 42229 28064 35348 651 x 10^{167}	50	49	0	6	9	12	14	16	18	19	19	20	[21]
110	2.14200 70197 90480 90232 50170 281 x 10^{188}	2.14200 70197 90480 90232 50439 819 x 10^{188}	51	51	0	6	10	13	15	17	19	20	21	22	22
120	1.41523 16756 71216 58447 27372 888 x 10^{209}	1.41523 16756 71216 58447 27373 741 x 10^{209}	51	51	0	7	10	13	16	18	20	22	23	24	25
130	2.06769 54720 42093 58405 38628 350 x 10^{230}	2.06769 54720 42093 58405 38628 356 x 10^{230}	51	51	0	7	10	14	17	19	22	24	25	26	27
140	6.30326 18392 06108 17159 58949 926 x 10^{251}	6.30326 18392 06108 17159 58949 926 x 10^{251}	51	51	0	7	11	14	18	20	23	25	27	28	29
150	3.81292 61315 81843 06671 95575 820 x 10^{273}	3.81292 61315 81843 06671 95575 820 x 10^{273}	51	51	0	7	11	15	18	21	24	26	28	30	30
	Excited state: n_2=0, m=1														
10	9.35031 68000 00000 00000 00000 000 x 10^{8}	1.11767 04000 00000 00000 00000 000 x 10^{9}	2	4	0	[1]	0								
20	1.07440 27756 35857 90894 08000 000 x 10^{22}	1.07396 06557 43091 91680 00000 000 x 10^{22}	8	7	0	2	[2]	1							
30	4.96521 64280 81112 14342 78197 278 x 10^{36}	4.96520 42172 87689 89982 16581 626 x 10^{36}	14	13	0	3	4	[4]	3	1					
40	3.99801 76984 58478 85839 30951 055 x 10^{52}	3.99801 78619 07896 89409 93296 235 x 10^{52}	19	19	0	4	5	6	[7]	6	4	2			
50	3.08017 19432 47631 67846 14925 771 x 10^{69}	3.08017 19430 76802 71994 53898 548 x 10^{69}	25	24	0	5	7	8	9	[10]	8	7	5	2	
60	1.51064 73927 65909 09148 07783 624 x 10^{87}	1.51064 73927 65876 63319 01487 744 x 10^{87}	30	29	0	5	8	9	11	11	[13]	11	10	8	6
70	3.54347 72322 61214 05011 24524 985 x 10^{105}	3.54347 72322 61214 36283 70471 596 x 10^{105}	35	34	0	6	8	11	12	13	14	[16]	14	13	12
80	3.22126 21010 05351 38105 57473 453 x 10^{124}	3.22126 21010 05351 38207 78748 772 x 10^{124}	40	39	0	6	9	12	14	15	16	17	[18]	17	16
90	9.66249 66725 03541 81258 59180 043 x 10^{143}	9.66249 66725 03541 81259 28362 982 x 10^{143}	45	44	0	6	10	13	15	17	18	19	19	[21]	19
100	8.42390 54522 94459 06273 21223 249 x 10^{163}	8.42390 54522 94459 06273 21336 172 x 10^{163}	50	50	0	7	10	13	16	18	20	21	22	22	[23]
110	1.92638 38811 73624 27229 46010 994 x 10^{184}	1.92638 38811 73624 27229 46011 479 x 10^{184}	51	51	0	7	11	14	17	19	21	23	24	25	25
120	1.06173 84185 01349 98205 76025 413 x 10^{205}	1.06173 84185 01349 98205 76025 414 x 10^{205}	51	51	0	7	11	15	18	21	23	25	26	27	27
130	1.31370 36327 74439 73620 80970 555 x 10^{226}	1.31370 36327 74439 73620 80970 555 x 10^{226}	51	51	0	7	12	15	19	22	24	26	28	29	30
140	3.43511 70363 70619 57753 36932 383 x 10^{247}	3.43511 70363 70619 57753 36932 383 x 10^{247}	51	51	0	7	12	16	19	22	25	27	29	30	30
150	1.80199 07698 85570 23304 01680 424 x 10^{269}	1.80199 07698 85570 23304 01680 424 x 10^{269}	51	51	0	8	12	16	20	23	26	29	30	30	30

TABLE IV. (*Continued*).

[a]Calculated by standard RSPT. Relative accuracy appears to be at least one part in 10^{29}.
[b]Calculated by the asymptotic formula, truncated at the value of k that gives a result closest to the exact value in the preceding column. This value of k is denoted by k_{best}.
[c]See b for definition of k_{best}. Generally, k_{best} increases with N. The "$k=51$" is not fundamentally significant in the sense that the maximum number of terms $c^{\{2\}(k)}$ available for this table was 51.
[d]The $k_{\min}$ is the value of k for which the term $c^{\{2\}(k)}/(N+4n_2+2m+1)\cdots(N+4n_2+2m+2-k)$ is smallest in magnitude, and which is a practical index for determining the truncation of the asymptotic formula.
[e]The number of significant figures in sum to k terms is operationally defined as the negative of the $\log_{10}$—truncated to an integer—of the magnitude of the relative error between the exact $\beta_2^{(N)}$ and the asymptotic formula. A box surrounds the entry on each line with the largest number of significant figures.

sum that comes closest to the exact result usually occurs when the last term is approximately the smallest. Compare the columns k_{best} and $k_{\min}$ in Table IV. The pattern of convergence followed by divergence is visible in the 11 rightmost columns of Table IV, in which are listed the approximate number of digits in the various partial sums that are the same as in the exact result. The best result is boxed.

The order at which the RSPT coefficients become asymptotic seems strongly dependent on n_2, more so than the corresponding n dependence for the anharmonic oscillator.[24] In particular, notice here that for the $(n_2=1, m=0)$ state, the best asymptotic value for $N=10$ does not even have the correct sign, while for the (0,0) and (0,1) states, for which n_2 is only 1 less, the errors in the best asymptotic values for the tenth-order coefficients are smaller than 2%. On the other hand, at the highest orders the accuracy obtained by using the asymptotic formula (229) is greater than the practical accuracy to which the RSPT calculation can be carried out.

IX. NUMERICAL CHARACTERIZATION OF THE β_1 SERIES

The asymptotics of the RSPT coefficients $\beta_1^{(N)}$ are more complicated than in the β_2 case because of the presence of small alternating-sign contributions, as in Eq. (197). First we list in Tables V–VIII the terms of the RSPT series, the induced exponentially small gap series $(\Delta\beta_1^{\{1\}})_{\text{ind}}$, and the induced doubly-exponentially-small imaginary series $(\Delta_i\beta_2^{\{2\}})_{\text{ind}}$, all through fifty-first order in $(2r)^{-1}$, for the ground state $(n_1=0, n_2=0, m=0)$ and for the three excited states for which n_1, n_2, and m are (1,0,0), (0,1,0), and (0,0,1). We use the notation $d^{\{1\}(N)}$ and $d^{\{2\}(N)}$ for the series coefficients for the two exponentially small quantities, according to

$$(\Delta\beta_1^{\{1\}})_{\text{ind}} = \mp 4\beta_1^{(0)} \frac{(2r)^{2\beta_2^{(0)}-1} e^{-r}}{n_2!(n_2+m)!} \times \sum_{N=0}^{\infty} d^{\{1\}(N)}(2r)^{-N}, \tag{230}$$

$$(\Delta_i\beta_1^{\{2\}})_{\text{ind}} = \pm \pi 4\beta_1^{(0)} \frac{(2r)^{4\beta_2^{(0)}-1} e^{-2r}}{[n_2!(n_2+m)!]^2} \times \sum_{N=0}^{\infty} d^{\{2\}(N)}(2r)^{-N} \quad (\pm \operatorname{Im} r \geq 0). \tag{231}$$

Notice that the coefficients (at least those with fewer than the maximum number of significant digits) appear to be integers, except in the (1,0,0) case for which multiplication of $d^{\{1\}(N)}$ and $d^{\{2\}(N)}$ by $4\beta_1^{(0)}$, which had been explicitly factored out in Eqs. (230) and (231) to make the leading coefficient of each power series equal to 1, is needed to restore the integer property of the coefficients. The coefficients are estimated to be accurate to the precision reported, with uncertainty only in the last digit. Notice that for the (0,1,0) state, only 27 digits have been reported for the coefficients $d^{\{1\}(N)}$ and $d^{\{2\}(N)}$, two fewer than the 29 reported for the other states. The lower accuracy comes from the lower accuracy of the $\Delta\beta_2$ quantities for $n_2=1$, as mentioned in Sec. VIII.

It is especially interesting to examine numerically the prediction of the asymptotics of the $\beta_1^{(N)}$ by the dispersion relation [Eqs. (196) and (197)], which in the notation of Eq. (231) becomes

$$\beta_1^{(N)} \sim 4\beta_1^{(0)} \frac{(N+4n_2+2m)!}{(n_2!)^2[(n_2+m)!]^2} \left[1 + \frac{d^{\{2\}(1)}}{N+4n_2+2m} + \frac{d^{\{2\}(2)}}{(N+4n_2+2m)(N+4n_2+2m-1)} + \cdots \right]$$
$$+ (-1)^{m+N-1} 16n^4 \frac{(n_1+2n_2+2m+1)!(n_1+2n_2+m+1)!}{n_1!(n_1+m)!} (N-4n_2-2m-5)!$$
$$\times \left[1 + \frac{4n^2 - 12(\beta_2^{(0)})^2 + m^2 - 1 + 12n - 12\beta_2^{(0)}}{N-4n_2-2m-5} \right.$$
$$- \frac{4n^2[2\psi(N-4n_2-2m-5) - \psi(n_1+2n_2+2m+2) - \psi(n_1+2n_2+m+2)]}{N-4n_2-2m-5}$$

TABLE V. Coefficients for the RSPT series, the induced $\Delta\beta_1^{\{1\}}$ series, and the induced $\Delta_i\beta_2^{\{2\}}$ series, as defined by Eqs. (24), (230), and (231) of the text, for the $(n_1=0, n_2=0, m=0)$ ground state of β_1.

Order N	$\beta_1^{(N)}$	Coefficient $d^{(1)(N)}$	$d^{(2)(N)}$
0	5.00000 00000 00000 00000 00000 000 × 10^{-1}	1.00000 00000 00000 00000 00000 000 × 10^{0}	1.00000 00000 00000 00000 00000 000 × 10^{0}
1	-1.00000 00000 00000 00000 00000 000 × 10^{0}	-4.00000 00000 00000 00000 00000 000 × 10^{0}	-6.00000 00000 00000 00000 00000 000 × 10^{0}
2	3.00000 00000 00000 00000 00000 000 × 10^{0}	-1.30000 00000 00000 00000 00000 000 × 10^{1}	-8.00000 00000 00000 00000 00000 000 × 10^{0}
3	4.00000 00000 00000 00000 00000 000 × 10^{0}	2.40000 00000 00000 00000 00000 000 × 10^{1}	4.80000 00000 00000 00000 00000 000 × 10^{1}
4	-1.50000 00000 00000 00000 00000 000 × 10^{1}	7.80000 00000 00000 00000 00000 000 × 10^{1}	3.50000 00000 00000 00000 00000 000 × 10^{1}
5	2.00000 00000 00000 00000 00000 000 × 10^{1}	-2.41600 00000 00000 00000 00000 000 × 10^{3}	-2.80200 00000 00000 00000 00000 000 × 10^{3}
6	6.70000 00000 00000 00000 00000 000 × 10^{2}	-1.44210 00000 00000 00000 00000 000 × 10^{4}	-1.24280 00000 00000 00000 00000 000 × 10^{4}
7	2.08800 00000 00000 00000 00000 000 × 10^{3}	-6.96400 00000 00000 00000 00000 000 × 10^{4}	-6.46800 00000 00000 00000 00000 000 × 10^{4}
8	1.52370 00000 00000 00000 00000 000 × 10^{4}	-1.35187 40000 00000 00000 00000 000 × 10^{6}	-1.50376 60000 00000 00000 00000 000 × 10^{6}
9	2.69124 00000 00000 00000 00000 000 × 10^{5}	-1.78985 76000 00000 00000 00000 000 × 10^{7}	-1.92010 04000 00000 00000 00000 000 × 10^{7}
10	2.88203 40000 00000 00000 00000 000 × 10^{6}	-2.12840 24600 00000 00000 00000 000 × 10^{8}	-2.30908 57600 00000 00000 00000 000 × 10^{8}
11	3.29663 60000 00000 00000 00000 000 × 10^{7}	-3.01974 30720 00000 00000 00000 000 × 10^{9}	-3.36538 88000 00000 00000 00000 000 × 10^{9}
12	4.47459 56200 00000 00000 00000 000 × 10^{8}	-4.54483 26068 00000 00000 00000 000 × 10^{10}	-5.12049 92481 00000 00000 00000 000 × 10^{10}
13	6.32327 70640 00000 00000 00000 000 × 10^{9}	-7.09487 44979 20000 00000 00000 000 × 10^{11}	-8.07869 01361 00000 00000 00000 000 × 10^{11}
14	9.41615 84444 00000 00000 00000 000 × 10^{10}	-1.17305 06423 68100 00000 00000 000 × 10^{13}	-1.35028 57256 35600 00000 00000 000 × 10^{13}
15	1.49465 94569 76000 00000 00000 000 × 10^{12}	-2.04480 29691 93520 00000 00000 000 × 10^{14}	-2.37556 62095 05200 00000 00000 000 × 10^{14}
16	2.50896 21727 14900 00000 00000 000 × 10^{13}	-3.74331 40151 12722 00000 00000 000 × 10^{15}	-4.38467 93150 69466 00000 00000 000 × 10^{15}
17	4.44107 76959 07560 00000 00000 000 × 10^{14}	-7.19022 18098 94692 80000 00000 000 × 10^{16}	-8.48500 32208 31374 80000 00000 000 × 10^{16}
18	8.27630 22888 56874 00000 00000 000 × 10^{15}	-1.44695 39118 25111 86600 00000 000 × 10^{18}	-1.71897 91414 53706 41600 00000 000 × 10^{18}
19	1.62043 42820 08490 16000 00000 000 × 10^{17}	-3.04574 24704 37673 96480 00000 000 × 10^{19}	-3.64027 70588 19622 76800 00000 000 × 10^{19}
20	3.32665 42683 11276 86200 00000 000 × 10^{18}	-6.69600 56582 50457 56508 00000 000 × 10^{20}	-8.04706 76187 70086 51282 00000 000 × 10^{20}
21	7.14803 50018 55492 32880 00000 000 × 10^{19}	-1.53530 78046 69211 58653 44000 000 × 10^{22}	-1.85431 01328 54897 47353 80000 000 × 10^{22}
22	1.60477 13847 23674 76739 60000 000 × 10^{21}	-3.66628 58198 97639 97890 61000 000 × 10^{23}	-4.44824 07790 72045 28938 58400 000 × 10^{23}
23	3.75822 42734 76225 74061 28000 000 × 10^{22}	-9.10589 61922 53374 11879 54080 000 × 10^{24}	-1.10941 02254 27301 64289 46896 000 × 10^{25}
24	9.16687 40607 24638 96645 79400 000 × 10^{23}	-2.34923 05463 98923 88120 44786 000 × 10^{26}	-2.87312 29928 32114 21853 87076 400 × 10^{26}
25	2.32541 05776 70704 11091 43656 000 × 10^{25}	-6.28779 53475 23274 79711 73328 960 × 10^{27}	-7.71710 75070 86905 96202 39138 160 × 10^{27}
26	6.12658 95311 81374 81240 87256 400 × 10^{26}	-1.74394 00617 97450 20708 54868 574 × 10^{29}	-2.14732 66220 20407 06871 05123 738 × 10^{29}
27	1.67424 38963 83292 13100 20687 472 × 10^{28}	-5.00654 90356 19520 14511 37306 079 × 10^{30}	-6.18316 65965 47777 29663 63569 926 × 10^{30}
28	4.73988 78827 63629 42618 53595 122 × 10^{29}	-1.48613 62899 68605 85578 94408 670 × 10^{32}	-1.84053 19599 33359 41159 96180 297 × 10^{32}
29	1.38857 46039 83325 69450 67309 963 × 10^{31}	-4.55672 98159 02719 24283 57532 163 × 10^{33}	-5.65804 24291 63796 53078 73498 596 × 10^{33}
30	4.20484 95981 43437 52856 90821 189 × 10^{32}	-1.44180 81565 73968 70724 02003 666 × 10^{35}	-1.79462 10504 91853 93537 76137 803 × 10^{35}
31	1.31482 83626 14689 16879 39208 591 × 10^{34}	-4.70355 49835 76415 28224 07054 869 × 10^{36}	-5.86780 11770 06854 85250 09353 278 × 10^{36}
32	4.24136 03481 22180 14997 27011 495 × 10^{35}	-1.58065 01348 46874 87815 29386 805 × 10^{38}	-1.97608 96485 24209 62107 26071 045 × 10^{38}
33	1.41014 46206 91339 49621 17275 387 × 10^{37}	-5.46739 04626 04654 62131 21114 989 × 10^{39}	-6.84882 80023 28656 58282 40344 683 × 10^{39}
34	4.82802 38503 08125 29553 31706 145 × 10^{38}	-1.94501 04865 38007 62705 89026 561 × 10^{41}	-2.44102 29561 68495 33074 11857 879 × 10^{41}
35	1.70085 93393 95120 27806 01785 581 × 10^{40}	-7.11114 88069 46235 45580 81940 492 × 10^{42}	-8.94038 83980 72800 63585 02213 994 × 10^{42}
36	6.16061 45090 62291 67417 63524 285 × 10^{41}	-2.67010 49290 24547 30646 82501 896 × 10^{44}	-3.36254 79378 11179 82704 72966 162 × 10^{44}
37	2.29254 43917 84602 54356 91615 649 × 10^{43}	-1.02895 47233 99288 02882 42885 648 × 10^{46}	-1.29783 76181 84014 23550 13409 900 × 10^{46}
38	8.75883 13712 37131 11125 90672 419 × 10^{44}	-4.06692 79816 39936 66719 31097 761 × 10^{47}	-5.13733 64427 31482 44532 59877 707 × 10^{47}
39	3.43337 61289 94263 40892 50487 074 × 10^{46}	-1.64768 45572 54938 84277 56459 764 × 10^{49}	-2.08429 60111 77635 95585 28134 552 × 10^{49}
40	1.37996 71455 77679 10787 76135 778 × 10^{48}	-6.83859 07906 54300 79662 87561 655 × 10^{50}	-8.66232 76799 88636 03867 60700 370 × 10^{50}
41	5.68364 56777 76939 56715 93198 012 × 10^{49}	-2.90604 57004 74733 80153 60140 153 × 10^{52}	-3.68573 65915 36765 44188 24983 761 × 10^{52}
42	2.39743 27759 27379 99597 60225 684 × 10^{51}	-1.26371 98945 70728 36639 32144 929 × 10^{54}	-1.60472 18947 32593 53788 29146 432 × 10^{54}
43	1.03511 60128 81049 75473 64800 434 × 10^{53}	-5.62070 16397 30529 07839 69701 964 × 10^{55}	-7.14565 00217 41842 95198 37721 847 × 10^{55}
44	4.57221 74033 53607 00487 72182 285 × 10^{54}	-2.55570 06965 13417 47071 75188 468 × 10^{57}	-3.25267 21114 85612 13205 48935 330 × 10^{57}
45	2.06510 55699 12521 40804 36906 726 × 10^{56}	-1.18742 45487 22635 93155 27883 184 × 10^{59}	-1.51284 28667 38801 32058 17295 744 × 10^{59}
46	9.53293 04351 29736 97591 97094 776 × 10^{57}	-5.63487 11230 95230 98226 15587 151 × 10^{60}	-7.18636 22223 28394 26339 10695 832 × 10^{60}
47	4.49551 59480 84994 45992 12875 709 × 10^{59}	-2.72996 27008 91040 66955 52909 076 × 10^{62}	-3.48497 99601 97580 60174 00095 153 × 10^{62}
48	2.16475 98108 65986 41705 01864 034 × 10^{61}	-1.34972 28597 45531 09158 35676 142 × 10^{64}	-1.72460 22071 31291 37859 01445 327 × 10^{64}
49	1.06397 86918 94291 98777 54647 453 × 10^{63}	-6.80729 73896 42091 66017 06788 314 × 10^{65}	-8.70569 08740 69746 26721 82341 450 × 10^{65}
50	5.33546 42871 48682 10315 34475 375 × 10^{64}	-3.50090 95278 72955 47800 21045 029 × 10^{67}	-4.48103 14973 89817 73962 23980 551 × 10^{67}
51	2.72871 13571 54325 27727 07900 166 × 10^{66}	-1.83528 22801 78086 38938 40031 805 × 10^{69}	-2.35100 70046 58677 98591 85924 876 × 10^{69}

$$+\frac{A(n_1,n_2,m)+8\pi^2 n^4/3+B(n_1,n_2,m)[\psi(N-4n_2-2m-6)-\psi(1)]}{(N-4n_2-2m-5)(N-4n_2-2m-6)}$$

$$+\,32n^4\frac{[\psi(N-4n_2-2m-6)-\psi(1)]^2+[\psi^{(1)}(N-4n_2-2m-6)-\psi^{(1)}(1)]}{(N-4n_2-2m-5)(N-4n_2-2m-6)}+O(N^{-3}(\ln N)^3)\Bigg]\,, \qquad (232)$$

TABLE VI. Coefficients for the RSPT series, the induced $\Delta\beta_1^{\{1\}}$ series, and the induced $\Delta_i\beta_1^{\{2\}}$ series, as defined by Eqs. (24), (230), and (231) of the text, for the $(n_1=1, n_2=0, m=0)$ excited state of β_1.

Order	Coefficient		
N	$\beta_1^{(N)}$	$d^{(1)(N)}$	$d^{(2)(N)}$
0	1. 50000 00000 00000 00000 00000 000 x 10^{0}	1. 00000 00000 00000 00000 00000 000 x 10^{0}	1. 00000 00000 00000 00000 00000 000 x 10^{0}
1	-7. 00000 00000 00000 00000 00000 000 x 10^{0}	-6. 66666 66666 66666 66666 66666 667 x 10^{0}	-8. 66666 66666 66666 66666 66666 667 x 10^{0}
2	4. 10000 00000 00000 00000 00000 000 x 10^{1}	-3. 16666 66666 66666 66666 66666 667 x 10^{1}	-2. 13333 33333 33333 33333 33333 333 x 10^{1}
3	-4. 40000 00000 00000 00000 00000 000 x 10^{1}	4. 93333 33333 33333 33333 33333 333 x 10^{2}	5. 62666 66666 66666 66666 66666 667 x 10^{2}
4	-1. 19300 00000 00000 00000 00000 000 x 10^{3}	1. 15000 00000 00000 00000 00000 000 x 10^{3}	2. 61666 66666 66666 66666 66666 667 x 10^{2}
5	6. 11600 00000 00000 00000 00000 000 x 10^{3}	-6. 23973 33333 33333 33333 33333 333 x 10^{4}	-6. 58340 00000 00000 00000 00000 000 x 10^{4}
6	7. 05620 00000 00000 00000 00000 000 x 10^{4}	1. 16248 33333 33333 33333 33333 333 x 10^{5}	2. 31964 00000 00000 00000 00000 000 x 10^{5}
7	-8. 29368 00000 00000 00000 00000 000 x 10^{5}	7. 72722 13333 33333 33333 33333 333 x 10^{6}	7. 62324 26666 66666 66666 66666 667 x 10^{6}
8	-3. 41667 70000 00000 00000 00000 000 x 10^{6}	-6. 18475 22000 00000 00000 00000 000 x 10^{7}	-7. 72888 00666 66666 66666 66666 667 x 10^{7}
9	1. 13068 88400 00000 00000 00000 000 x 10^{8}	-8. 42283 16000 00000 00000 00000 000 x 10^{8}	-7. 43142 97733 33333 33333 33333 333 x 10^{8}
10	-1. 79195 28200 00000 00000 00000 000 x 10^{8}	1. 46442 37396 66666 66666 66666 667 x 10^{10}	1. 63754 50149 33333 33333 33333 333 x 10^{10}
11	-1. 34513 82472 00000 00000 00000 000 x 10^{10}	3. 43071 41936 00000 00000 00000 000 x 10^{10}	7. 18175 56746 66666 66666 66666 667 x 10^{9}
12	1. 09344 37922 20000 00000 00000 000 x 10^{11}	-2. 73967 41295 98666 66666 66666 667 x 10^{12}	-2. 84917 31128 25000 00000 00000 000 x 10^{12}
13	1. 21222 07307 28000 00000 00000 000 x 10^{12}	1. 27609 49047 87733 33333 33333 333 x 10^{13}	1. 78532 34072 04600 00000 00000 000 x 10^{13}
14	-2. 34834 55342 78000 00000 00000 000 x 10^{13}	3. 50924 53122 81990 00000 00000 000 x 10^{14}	3. 29713 35833 86813 33333 33333 333 x 10^{14}
15	-6. 64147 48099 68000 00000 00000 000 x 10^{12}	-5. 21041 31435 67269 33333 33333 333 x 10^{15}	-5. 96872 95618 82021 33333 33333 333 x 10^{15}
16	3. 68198 03876 95443 00000 00000 000 x 10^{15}	-2. 53405 07211 42271 66666 66666 667 x 10^{16}	-1. 68740 75926 99814 86666 66666 667 x 10^{16}
17	-2. 42694 33864 25159 60000 00000 000 x 10^{16}	9. 88591 33706 46110 80000 00000 000 x 10^{17}	1. 03249 05058 03139 08400 00000 000 x 10^{18}
18	-3. 40561 99793 92368 74000 00000 000 x 10^{17}	-5. 91101 62495 79187 25800 00000 000 x 10^{18}	-8. 12990 29387 30036 64000 00000 000 x 10^{18}
19	7. 09501 97360 50132 44000 00000 000 x 10^{18}	-1. 66998 41800 96913 91504 00000 000 x 10^{20}	-1. 65251 97880 79554 23269 33333 333 x 10^{20}
20	1. 16915 00241 71507 44340 00000 000 x 10^{19}	1. 41744 91463 50752 99518 26666 667 x 10^{21}	1. 58760 39756 82137 42742 20000 000 x 10^{21}
21	-8. 81265 96450 72444 92872 00000 000 x 10^{20}	-5. 56501 87521 77884 73026 66666 666 x 10^{21}	-1. 18582 44364 69751 65837 48000 000 x 10^{22}
22	1. 20751 60057 96617 85615 00000 000 x 10^{22}	-7. 16663 11501 81188 25418 28466 667 x 10^{23}	-8. 03525 14474 24689 17412 33866 667 x 10^{23}
23	1. 97949 89310 65092 63420 91200 000 x 10^{23}	-5. 78042 75533 53166 32533 79840 000 x 10^{24}	-6. 74806 16793 35118 93178 77333 333 x 10^{24}
24	3. 26013 25212 39662 02953 56599 999 x 10^{23}	-1. 54293 83915 45296 33570 65315 067 x 10^{26}	-2. 03365 30320 00410 56577 75020 933 x 10^{26}
25	6. 15097 96937 35826 99326 82760 000 x 10^{25}	-6. 28071 67981 19877 21247 12644 960 x 10^{27}	-7. 64122 21966 67400 09200 60580 293 x 10^{27}
26	1. 92118 08535 14465 11744 90460 920 x 10^{27}	-1. 55442 04421 44982 18418 25633 240 x 10^{29}	-1. 89718 52844 56940 23490 18679 820 x 10^{29}
27	4. 15473 29342 15424 88507 72395 568 x 10^{28}	-4. 28157 92804 15504 43335 75287 735 x 10^{30}	-5. 32122 19424 87547 24371 08386 214 x 10^{30}
28	1. 22975 30198 68885 90077 25825 155 x 10^{30}	-1. 32939 23829 17679 54615 36481 879 x 10^{32}	-1. 64832 21478 16887 52799 75278 894 x 10^{32}
29	3. 76389 92476 17554 97550 20396 163 x 10^{31}	-4. 08341 21033 98877 37883 71430 426 x 10^{33}	-5. 06825 60499 48340 72030 31922 927 x 10^{33}
30	1. 12470 40077 84147 09191 26189 480 x 10^{33}	-1. 28888 58471 97819 83522 99974 850 x 10^{35}	-1. 60565 88891 13306 34501 41482 892 x 10^{35}
31	3. 52426 22803 36178 07278 53762 966 x 10^{34}	-4. 22967 71850 19734 28452 66515 917 x 10^{36}	-5. 28036 47481 68471 56190 98295 781 x 10^{36}
32	1. 14509 25465 07593 34240 09922 211 x 10^{36}	-1. 42715 05169 04092 29520 13118 295 x 10^{38}	-1. 78503 74027 81790 89105 75054 942 x 10^{38}
33	3. 81870 52287 55575 04208 17372 653 x 10^{37}	-4. 95079 02261 69961 98770 02705 393 x 10^{39}	-6. 20479 76531 90347 86246 40312 857 x 10^{39}
34	1. 31138 31610 02830 25514 44561 739 x 10^{39}	-1. 76685 55955 97570 54904 12681 767 x 10^{41}	-2. 21848 93047 47486 84579 77978 139 x 10^{41}
35	4. 63527 95548 81703 42107 57979 025 x 10^{40}	-6. 47936 62869 79387 92773 32935 212 x 10^{42}	-8. 14960 30888 19988 79134 49715 844 x 10^{42}
36	1. 68397 18149 95061 54938 41790 695 x 10^{42}	-2. 43968 53680 85297 45434 43318 711 x 10^{44}	-3. 07361 22533 12747 37997 19045 305 x 10^{44}
37	6. 28413 68274 68655 29873 69117 033 x 10^{43}	-9. 42659 54737 00890 76943 68986 191 x 10^{45}	-1. 18944 11294 93893 42292 68364 024 x 10^{46}
38	2. 40732 62624 95121 58317 30959 517 x 10^{45}	-3. 73524 32862 92268 32303 64578 464 x 10^{47}	-4. 72001 88009 45974 02065 18571 093 x 10^{47}
39	9. 46037 67189 73453 98270 12646 060 x 10^{46}	-1. 51692 02235 85775 30525 33352 513 x 10^{49}	-1. 91951 59080 15736 62417 05578 442 x 10^{49}
40	3. 81149 49519 09701 02495 76615 853 x 10^{48}	-6. 31013 44694 47637 47524 37046 491 x 10^{50}	-7. 99542 40832 01651 23761 28846 358 x 10^{50}
41	1. 57340 44239 91749 11825 05650 717 x 10^{50}	-2. 68725 67307 04044 83977 64280 558 x 10^{52}	-3. 40924 20085 10290 08938 00650 007 x 10^{52}
42	6. 65115 23979 40872 72589 32947 434 x 10^{51}	-1. 17097 17122 10135 02095 14213 719 x 10^{54}	-1. 48735 55373 75308 07083 86056 362 x 10^{54}
43	2. 87760 16315 26658 55137 53854 547 x 10^{53}	-5. 21834 33559 83625 90180 83838 383 x 10^{55}	-6. 63584 86522 20168 59775 35831 723 x 10^{55}
44	1. 27355 17426 99160 79925 99461 395 x 10^{55}	-2. 37716 19273 03823 97663 68418 574 x 10^{57}	-3. 02618 45821 84015 35826 92686 848 x 10^{57}
45	5. 76288 84684 97828 21323 99269 039 x 10^{56}	-1. 10643 14593 67734 27399 83948 857 x 10^{59}	-1. 40997 97023 30513 80341 05193 571 x 10^{59}
46	2. 66498 66877 42796 23929 86432 775 x 10^{58}	-5. 25941 35460 63484 80773 24744 773 x 10^{60}	-6. 70899 76276 90323 31483 78517 771 x 10^{60}
47	1. 25887 91199 86255 29617 78445 987 x 10^{60}	-2. 55218 69946 65667 82546 43291 314 x 10^{62}	-3. 25871 43206 69375 06791 54046 356 x 10^{62}
48	6. 07179 59383 97913 80942 15037 690 x 10^{61}	-1. 26378 20620 84775 64357 76979 738 x 10^{64}	-1. 61511 01709 81924 00820 30224 571 x 10^{64}
49	2. 98890 97959 38819 27707 38732 468 x 10^{63}	-6. 38330 46488 82303 07864 73303 599 x 10^{65}	-8. 16498 57475 89338 04235 55360 497 x 10^{65}
50	1. 50105 14192 52281 88217 50777 945 x 10^{65}	-3. 28751 66731 79286 06794 79285 017 x 10^{67}	-4. 20864 64045 76984 29032 05797 188 x 10^{67}
51	7. 68771 90349 10869 47644 32034 197 x 10^{66}	-1. 72576 20869 67645 27532 23739 782 x 10^{69}	-2. 21108 59288 93518 33482 72601 500 x 10^{69}

where the coefficients $A(n_1,n_2,m)$ and $B(n_1,n_2,m)$, which are independent of N, are given for the first few states in Table IX. The $\psi^{(1)}(z)$ denotes the digamma function,

$$\psi^{(1)}(z) = d\psi(z)/dz = d^2[\ln\Gamma(z)]/dz^2 \ . \qquad (233)$$

In Table X we uncover numerically the alternating-sign contributions to the asymptotics by subtracting the terms in Eq. (233) that come from $(\Delta_i\beta_1^{\{2\}})_{\rm ind}$ (those involving the coefficients $d^{\{2\}(k)}$). We truncate the partial sum after including the smallest term. Listed in Table X are the exact $\beta_1^{(N)}$, the k index of the last correction term included in the partial sum and the value of that term, the difference between the exact and asymptotic values—divided by

TABLE VII. Coefficients for the RSPT series, the induced $\Delta\beta_1^{[1]}$ series, and the induced $\Delta_i\beta_1^{[2]}$ series, as defined by Eqs. (24), (230), and (231) of the text, for the $(n_1=0,n_2=1,m=0)$ excited state of β_1.

Order N	Coefficient $\beta_1^{(N)}$	$d^{(1)(N)}$	$d^{(2)(N)}$
0	5.00000 00000 00000 00000 00000 000 $\times 10^{-1}$	1.00000 00000 00000 00000 00000 0 $\times 10^{0}$	1.00000 00000 00000 00000 00000 0 $\times 10^{0}$
1	-3.00000 00000 00000 00000 00000 000 $\times 10^{0}$	-1.60000 00000 00000 00000 00000 0 $\times 10^{1}$	-3.00000 00000 00000 00000 00000 0 $\times 10^{1}$
2	7.00000 00000 00000 00000 00000 000 $\times 10^{0}$	-1.10000 00000 00000 00000 00000 0 $\times 10^{1}$	2.36000 00000 00000 00000 00000 0 $\times 10^{2}$
3	7.60000 00000 00000 00000 00000 000 $\times 10^{1}$	3.60000 00000 00000 00000 00000 0 $\times 10^{1}$	-2.72000 00000 00000 00000 00000 0 $\times 10^{2}$
4	4.73000 00000 00000 00000 00000 000 $\times 10^{2}$	1.85900 00000 00000 00000 00000 0 $\times 10^{3}$	1.15700 00000 00000 00000 00000 0 $\times 10^{3}$
5	2.20400 00000 00000 00000 00000 000 $\times 10^{3}$	-8.10400 00000 00000 00000 00000 0 $\times 10^{3}$	-3.33660 00000 00000 00000 00000 0 $\times 10^{4}$
6	2.45420 00000 00000 00000 00000 000 $\times 10^{4}$	-7.32858 00000 00000 00000 00000 0 $\times 10^{5}$	-6.07552 00000 00000 00000 00000 0 $\times 10^{5}$
7	5.88216 00000 00000 00000 00000 000 $\times 10^{5}$	-1.53358 16000 00000 00000 00000 0 $\times 10^{7}$	-6.43637 60000 00000 00000 00000 0 $\times 10^{6}$
8	1.15534 45000 00000 00000 00000 000 $\times 10^{7}$	-2.63817 19300 00000 00000 00000 0 $\times 10^{8}$	-9.46010 89000 00000 00000 00000 0 $\times 10^{7}$
9	1.99186 09200 00000 00000 00000 000 $\times 10^{8}$	-5.27898 58240 00000 00000 00000 0 $\times 10^{9}$	-2.57506 07700 00000 00000 00000 0 $\times 10^{9}$
10	3.58753 16660 00000 00000 00000 000 $\times 10^{9}$	-1.22518 92719 40000 00000 00000 0 $\times 10^{11}$	-6.94628 38292 00000 00000 00000 0 $\times 10^{10}$
11	7.12503 04712 00000 00000 00000 000 $\times 10^{10}$	-2.92458 45919 28000 00000 00000 0 $\times 10^{12}$	-1.69282 38371 52000 00000 00000 0 $\times 10^{12}$
12	1.50188 07901 86000 00000 00000 000 $\times 10^{12}$	-7.00612 38516 15800 00000 00000 0 $\times 10^{13}$	-4.10705 37222 23800 00000 00000 0 $\times 10^{13}$
13	3.27019 82442 13600 00000 00000 000 $\times 10^{13}$	-1.71634 61686 62416 00000 00000 0 $\times 10^{15}$	-1.03799 71906 87804 00000 00000 0 $\times 10^{15}$
14	7.35183 87955 93560 00000 00000 000 $\times 10^{14}$	-4.33566 00299 36582 80000 00000 0 $\times 10^{16}$	-2.71321 51854 76465 60000 00000 0 $\times 10^{16}$
15	1.71157 82914 66660 80000 00000 000 $\times 10^{16}$	-1.12642 04094 27557 07200 00000 0 $\times 10^{18}$	-7.25861 96252 52186 40000 00000 0 $\times 10^{17}$
16	4.12157 16112 31827 65000 00000 000 $\times 10^{17}$	-3.00212 07586 55063 15410 00000 0 $\times 10^{19}$	-1.98571 92375 00830 26130 00000 0 $\times 10^{19}$
17	1.02434 70197 19986 60600 00000 000 $\times 10^{19}$	-8.20472 28370 77264 74512 00000 0 $\times 10^{20}$	-5.56286 69144 26918 07690 00000 0 $\times 10^{20}$
18	2.62424 97627 20094 94538 00000 000 $\times 10^{20}$	-2.29954 72976 55993 55852 90000 0 $\times 10^{22}$	-1.59637 90374 37729 53291 32000 0 $\times 10^{22}$
19	6.92538 54395 74197 44311 20000 000 $\times 10^{21}$	-6.60875 46363 32434 31188 24800 0 $\times 10^{23}$	-4.69193 48278 39251 52204 56000 0 $\times 10^{23}$
20	1.88159 56375 04565 96826 75000 000 $\times 10^{23}$	-1.94730 33237 03558 56981 86066 0 $\times 10^{25}$	-1.41226 02958 55028 55237 24914 0 $\times 10^{25}$
21	5.26069 16904 99237 79536 28880 000 $\times 10^{24}$	-5.88228 08612 96398 90851 60596 8 $\times 10^{26}$	-4.35344 24560 09007 63297 15101 2 $\times 10^{26}$
22	1.51293 29457 82333 19589 77795 600 $\times 10^{26}$	-1.82150 55926 13047 33772 85523 0 $\times 10^{28}$	-1.37439 96748 17561 34582 60723 5 $\times 10^{28}$
23	4.47414 01342 76342 64495 53986 720 $\times 10^{27}$	-5.78177 82459 83323 41812 01689 1 $\times 10^{29}$	-4.44376 84615 76293 49221 30142 0 $\times 10^{29}$
24	1.36012 57090 58448 64003 87781 443 $\times 10^{29}$	-1.88107 21862 51768 19988 56712 4 $\times 10^{31}$	-1.47140 89405 83249 42865 26866 8 $\times 10^{31}$
25	4.24912 38126 88853 45787 73952 599 $\times 10^{30}$	-6.27220 10831 94372 87878 32447 5 $\times 10^{32}$	-4.98921 95028 83656 84990 51092 9 $\times 10^{32}$
26	1.36376 99128 75067 39407 01023 402 $\times 10^{32}$	-2.14313 97789 29072 87061 18873 4 $\times 10^{34}$	-1.73224 48305 62366 72198 85388 2 $\times 10^{34}$
27	4.49541 85682 10455 46472 63013 143 $\times 10^{33}$	-7.50290 31849 57311 71342 16249 3 $\times 10^{35}$	-6.15756 99731 63269 51537 61930 2 $\times 10^{35}$
28	1.52140 71592 38878 96045 67931 230 $\times 10^{35}$	-2.69076 14480 47055 87220 26024 5 $\times 10^{37}$	-2.24060 22086 96186 78737 78186 3 $\times 10^{37}$
29	5.28467 15512 36667 88595 75075 701 $\times 10^{36}$	-9.88310 79544 33969 04507 72181 1 $\times 10^{38}$	-8.34437 94041 44198 83888 04852 0 $\times 10^{38}$
30	1.88334 79843 92160 98539 04706 216 $\times 10^{38}$	-3.71687 22699 60920 88735 20085 7 $\times 10^{40}$	-3.17982 74915 14242 22242 27842 8 $\times 10^{40}$
31	6.88364 51840 29576 27236 56430 660 $\times 10^{39}$	-1.43090 21471 40646 68397 44812 4 $\times 10^{42}$	-1.23962 09173 29935 85986 91713 5 $\times 10^{42}$
32	2.57935 21900 02766 31409 31923 341 $\times 10^{41}$	-5.63720 30878 95206 87404 96219 8 $\times 10^{43}$	-4.94238 35747 05747 99400 68339 3 $\times 10^{43}$
33	9.90446 48234 20972 19338 80297 117 $\times 10^{42}$	-2.27198 06644 33492 85026 06632 1 $\times 10^{45}$	-2.01476 80336 03267 59953 27464 7 $\times 10^{45}$
34	3.89583 00598 59278 99861 66241 170 $\times 10^{44}$	-9.36467 56365 68936 33564 11383 7 $\times 10^{46}$	-8.39513 27726 98622 27360 48169 3 $\times 10^{46}$
35	1.56904 71125 19523 88830 98567 601 $\times 10^{46}$	-3.94624 22600 40202 03825 69350 8 $\times 10^{48}$	-3.57447 58295 46803 80449 80418 6 $\times 10^{48}$
36	6.46780 04383 22177 60983 23330 043 $\times 10^{47}$	-1.69953 68815 05508 44788 49297 2 $\times 10^{50}$	-1.55469 30023 77696 61790 98848 9 $\times 10^{50}$
37	2.72759 58567 26769 65576 05805 592 $\times 10^{49}$	-7.47798 70543 94860 03838 19688 5 $\times 10^{51}$	-6.90538 06752 21001 36018 40912 1 $\times 10^{51}$
38	1.17632 09503 68074 33933 05565 329 $\times 10^{51}$	-3.36044 69139 49031 58016 25038 4 $\times 10^{53}$	-3.13114 76417 84381 12689 93059 2 $\times 10^{53}$
39	5.18580 22925 69076 99152 89133 741 $\times 10^{52}$	-1.54176 77215 37580 87487 55089 8 $\times 10^{55}$	-1.44895 36974 60787 21752 55337 6 $\times 10^{55}$
40	2.33601 29632 88540 34686 03844 720 $\times 10^{54}$	-7.21943 04199 76172 71275 61786 6 $\times 10^{56}$	-6.84074 12754 02706 37451 18826 4 $\times 10^{56}$
41	1.07481 07355 18888 10286 39238 594 $\times 10^{56}$	-3.44907 93995 45493 55225 13672 0 $\times 10^{58}$	-3.29392 18626 44321 64684 19958 2 $\times 10^{58}$
42	5.04914 98739 45764 19114 11397 049 $\times 10^{57}$	-1.68064 52537 51663 22973 95316 2 $\times 10^{60}$	-1.61714 97003 01863 59069 86553 9 $\times 10^{60}$
43	2.42086 25611 74634 93479 28437 857 $\times 10^{59}$	-8.34988 16823 33922 62150 65013 9 $\times 10^{61}$	-8.09247 19511 97967 51152 59699 3 $\times 10^{61}$
44	1.18420 76673 22064 89336 55536 184 $\times 10^{61}$	-4.22841 41006 42764 41662 88191 1 $\times 10^{63}$	-4.12644 10065 18375 08391 53343 4 $\times 10^{63}$
45	5.90793 85637 45149 24753 04073 134 $\times 10^{62}$	-2.18188 58441 45653 68791 98808 3 $\times 10^{65}$	-2.14341 03255 98137 49274 17318 9 $\times 10^{65}$
46	3.00499 12592 94226 08574 01435 798 $\times 10^{64}$	-1.14686 22369 21255 27935 70489 3 $\times 10^{67}$	-1.13382 10736 83294 68910 78415 7 $\times 10^{67}$
47	1.55776 74229 43548 10705 53484 823 $\times 10^{66}$	-6.13883 06655 24239 74139 48667 7 $\times 10^{68}$	-6.10618 77092 76137 44056 96316 6 $\times 10^{68}$
48	8.22756 64307 51413 82854 65427 712 $\times 10^{67}$	-3.34525 15267 84437 60764 35124 6 $\times 10^{70}$	-3.34704 65424 72815 14960 39210 2 $\times 10^{70}$
49	4.42599 46484 79762 08813 37494 638 $\times 10^{69}$	-1.85531 33466 22017 11678 58337 7 $\times 10^{72}$	-1.86681 62659 81557 41120 72547 9 $\times 10^{72}$
50	2.42430 03916 44025 05264 53488 183 $\times 10^{71}$	-1.04696 18292 31769 77372 32974 1 $\times 10^{74}$	-1.05919 17211 63757 51686 52725 0 $\times 10^{74}$
51	1.35165 95277 13310 09839 94743 745 $\times 10^{73}$	-6.00969 28536 88763 00572 36191 0 $\times 10^{75}$	-6.11178 96856 09539 41313 76803 3 $\times 10^{75}$

the leading asymptotic term (called the relative asymptotic error in the table), and the relative asymptotic error after taking account of one, two, and three terms from the alternating-sign asymptotic formula. These quantities are listed for various orders, up to order 150.

Notice that for the ground state the residual remaining after subtraction of the same-sign terms is alternating in sign after order $N=32$, and that it has relative magnitude 10^{-10} at order 150—which is small compared to unity, but large compared with the corresponding relative residual for $\beta_2^{(N)}$, which at order 110 is already less than 10^{-30}. The first alternating-sign asymptotic contribution significantly overcompensates, but by the third alternating-sign contribution the relative error has dropped by a factor of 10^{-3} at $N=150$ (see Table X).

For the excited states, the threshold for alternation is

TABLE VIII. Coefficients for the RSPT series, the induced $\Delta\beta_1^{(1)}$ series, and the induced $\Delta_i\beta_1^{(2)}$ series, as defined by Eqs. (24), (230), and (231) of the text, for the ($n_1=0, n_2=0, m=1$) excited state of β_1.

Order N	Coefficient $\beta_1^{(N)}$	$d^{(1)(N)}$	$d^{(2)(N)}$
0	1.00000 00000 00000 00000 00000 000 x 10^{0}	1.00000 00000 00000 00000 00000 000 x 10^{0}	1.00000 00000 00000 00000 00000 000 x 10^{0}
1	-6.00000 00000 00000 00000 00000 000 x 10^{0}	-9.00000 00000 00000 00000 00000 000 x 10^{0}	-1.50000 00000 00000 00000 00000 000 x 10^{1}
2	2.00000 00000 00000 00000 00000 000 x 10^{1}	-3.60000 00000 00000 00000 00000 000 x 10^{1}	1.40000 00000 00000 00000 00000 000 x 10^{1}
3	7.20000 00000 00000 00000 00000 000 x 10^{1}	1.68000 00000 00000 00000 00000 000 x 10^{2}	3.72000 00000 00000 00000 00000 000 x 10^{2}
4	-2.96000 00000 00000 00000 00000 000 x 10^{2}	2.88400 00000 00000 00000 00000 000 x 10^{3}	1.96800 00000 00000 00000 00000 000 x 10^{3}
5	-2.97600 00000 00000 00000 00000 000 x 10^{3}	-1.67160 00000 00000 00000 00000 000 x 10^{4}	-3.41520 00000 00000 00000 00000 000 x 10^{4}
6	2.46400 00000 00000 00000 00000 000 x 10^{4}	-4.65200 00000 00000 00000 00000 000 x 10^{5}	-3.87488 00000 00000 00000 00000 000 x 10^{5}
7	3.71712 00000 00000 00000 00000 000 x 10^{5}	-8.39280 00000 00000 00000 00000 000 x 10^{5}	1.66396 80000 00000 00000 00000 000 x 10^{6}
8	-2.25760 00000 00000 00000 00000 000 x 10^{5}	2.18013 12000 00000 00000 00000 000 x 10^{7}	2.41559 52000 00000 00000 00000 000 x 10^{7}
9	-1.27848 96000 00000 00000 00000 000 x 10^{7}	-4.17311 71200 00000 00000 00000 000 x 10^{8}	-6.01960 36800 00000 00000 00000 000 x 10^{8}
10	3.37753 98400 00000 00000 00000 000 x 10^{8}	-1.20459 12192 00000 00000 00000 000 x 10^{10}	-1.07949 72000 00000 00000 00000 000 x 10^{10}
11	6.29207 80800 00000 00000 00000 000 x 10^{9}	-1.11054 41817 60000 00000 00000 000 x 10^{11}	-6.17923 47840 00000 00000 00000 000 x 10^{10}
12	4.46035 53024 00000 00000 00000 000 x 10^{10}	-1.49466 42764 16000 00000 00000 000 x 10^{12}	-1.24621 59482 88000 00000 00000 000 x 10^{12}
13	7.15418 32089 60000 00000 00000 000 x 10^{11}	-4.48421 16789 69600 00000 00000 000 x 10^{13}	-4.45028 21904 00000 00000 00000 000 x 10^{13}
14	2.03911 95740 16000 00000 00000 000 x 10^{13}	-9.83228 35735 52640 00000 00000 000 x 10^{14}	-9.00756 33791 33440 00000 00000 000 x 10^{14}
15	3.91597 65915 64800 00000 00000 000 x 10^{14}	-1.85692 24673 25772 80000 00000 000 x 10^{16}	-1.67195 75006 63654 40000 00000 000 x 10^{16}
16	6.96322 20405 08928 00000 00000 000 x 10^{15}	-4.01464 36322 76270 08000 00000 000 x 10^{17}	-3.80769 86293 01468 16000 00000 000 x 10^{17}
17	1.46605 53194 98629 12000 00000 000 x 10^{17}	-9.46012 45723 67989 24800 00000 000 x 10^{18}	-9.17003 67331 94049 02400 00000 000 x 10^{18}
18	3.29272 11924 03306 49600 00000 000 x 10^{18}	-2.23320 58433 09975 36768 00000 000 x 10^{20}	-2.17689 35595 90026 08640 00000 000 x 10^{20}
19	7.40730 32159 32305 40800 00000 000 x 10^{19}	-5.40352 14885 93695 77267 20000 000 x 10^{21}	-5.33572 67800 95879 02668 80000 000 x 10^{21}
20	1.72561 16432 82305 15916 80000 000 x 10^{21}	-1.36437 79028 23278 43743 74400 000 x 10^{23}	-1.36710 90561 57953 16219 90400 000 x 10^{23}
21	4.20880 66125 03693 22352 64000 000 x 10^{22}	-3.56771 47632 05346 92466 89280 000 x 10^{24}	-3.61694 68087 31243 86955 67360 000 x 10^{24}
22	1.06438 80878 57307 70655 64160 000 x 10^{24}	-9.62363 70434 66291 72383 66208 000 x 10^{25}	-9.86029 61822 99713 08328 55040 000 x 10^{25}
23	2.78393 13703 71200 11050 02496 000 x 10^{25}	-2.68089 98759 50788 22605 89199 360 x 10^{27}	-2.77518 47502 25593 04511 45687 040 x 10^{27}
24	7.53852 00041 68339 87337 86316 800 x 10^{26}	-7.71195 72340 42472 84314 97265 152 x 10^{28}	-8.06032 89809 48260 83524 83905 536 x 10^{28}
25	2.11198 76904 88910 99508 67046 400 x 10^{28}	-2.28861 33721 35542 53994 10402 755 x 10^{30}	-2.41344 41537 00352 81655 60085 176 x 10^{30}
26	6.11464 65872 55323 40683 39523 584 x 10^{29}	-7.00170 66012 65845 26038 53523 976 x 10^{31}	-7.44555 57545 58028 51011 01329 211 x 10^{31}
27	1.82797 96604 62615 88022 55010 857 x 10^{31}	-2.20700 93799 04238 39769 51855 376 x 10^{33}	-2.36537 72213 61303 19132 05487 849 x 10^{33}
28	5.63852 03255 91947 05247 64528 640 x 10^{32}	-7.16299 43060 34201 28929 77653 586 x 10^{34}	-7.73360 48344 22401 45356 56815 643 x 10^{34}
29	1.79312 47384 82091 52262 65275 347 x 10^{34}	-2.39217 16874 59205 51969 91700 407 x 10^{36}	-2.60061 25445 47291 12371 87170 248 x 10^{36}
30	5.87451 48992 96768 23194 89954 723 x 10^{35}	-8.21525 55000 34653 27540 43155 874 x 10^{37}	-8.98920 26054 14045 09471 12333 781 x 10^{37}
31	1.98119 32373 63998 58121 55427 092 x 10^{37}	-2.89940 92932 46504 76441 02995 823 x 10^{39}	-3.19198 92003 63830 27048 95663 515 x 10^{39}
32	6.87325 20735 84420 35294 02226 527 x 10^{38}	-1.05097 34607 02630 44992 05085 627 x 10^{41}	-1.16370 61845 89977 27611 21056 789 x 10^{41}
33	2.45118 34082 97553 95324 88815 077 x 10^{40}	-3.91028 47723 82726 92217 39085 949 x 10^{42}	-4.35330 85697 95494 62054 68953 708 x 10^{42}
34	8.97998 82196 75969 55623 82117 975 x 10^{41}	-1.49247 59671 91028 47855 01526 589 x 10^{44}	-1.67012 29776 37649 12978 13267 411 x 10^{44}
35	3.37739 10182 51818 55680 08871 467 x 10^{43}	-5.84042 04860 89666 09999 73313 066 x 10^{45}	-6.56743 30633 07798 27704 63949 694 x 10^{45}
36	1.30323 41503 40617 71793 17227 595 x 10^{45}	-2.34197 33079 60815 58421 88893 972 x 10^{47}	-2.64565 52721 49439 17631 61585 426 x 10^{47}
37	5.15631 55948 30872 56299 21925 933 x 10^{46}	-9.61815 74995 36974 88794 25465 360 x 10^{48}	-1.09129 06998 01908 92295 09961 828 x 10^{49}
38	2.09065 82562 58745 50515 57167 087 x 10^{48}	-4.04345 64385 16972 65290 03940 175 x 10^{50}	-4.60684 37915 84883 54396 05309 551 x 10^{50}
39	8.68187 52142 23307 11183 62797 430 x 10^{49}	-1.73920 60891 88114 13144 90475 746 x 10^{52}	-1.98936 99758 47439 27652 31344 784 x 10^{52}
40	3.69063 26675 18006 00208 60429 351 x 10^{51}	-7.65033 79882 36403 00791 15754 417 x 10^{53}	-8.78368 46027 07649 53056 63673 097 x 10^{53}
41	1.60518 01749 19566 75006 47462 211 x 10^{53}	-3.43987 47287 25057 07624 64147 698 x 10^{55}	-3.96363 59968 50718 39338 07890 750 x 10^{55}
42	7.13953 55081 81224 56795 12009 987 x 10^{54}	-1.58032 05317 54483 47365 57341 989 x 10^{57}	-1.82717 40290 18809 47226 51926 710 x 10^{57}
43	3.24589 95781 17038 85425 61729 472 x 10^{56}	-7.41486 32510 73020 13385 05689 433 x 10^{58}	-8.60111 47974 09253 37993 68754 721 x 10^{58}
44	1.50772 70549 53703 73005 42506 269 x 10^{58}	-3.55171 28658 38617 24523 02337 713 x 10^{60}	-4.13279 53435 36142 71584 33200 534 x 10^{60}
45	7.15227 04422 62387 82302 78905 417 x 10^{59}	-1.73610 83866 30573 56724 54188 635 x 10^{62}	-2.02618 40080 46676 34647 15810 363 x 10^{62}
46	3.46351 27027 92517 52568 83207 133 x 10^{61}	-8.65672 46881 41991 49853 13887 812 x 10^{63}	-1.01320 38574 82571 76908 11616 640 x 10^{64}
47	1.71145 75733 99702 90564 51859 238 x 10^{63}	-4.40156 74704 32062 42241 23152 691 x 10^{65}	-5.16583 23267 77131 18550 99552 836 x 10^{65}
48	8.62627 34972 23210 78390 48989 304 x 10^{64}	-2.28130 19298 15868 74203 94559 384 x 10^{67}	-2.68446 06615 27810 01250 47682 301 x 10^{67}
49	4.43328 20579 38699 70577 93143 863 x 10^{66}	-1.20484 08918 78608 36066 66226 948 x 10^{69}	-1.42134 58961 00771 32425 47090 578 x 10^{69}
50	2.32228 57781 67440 81308 76905 700 x 10^{68}	-6.48191 04733 54002 05926 80356 188 x 10^{70}	-7.66524 46235 73762 00834 94081 407 x 10^{70}
51	1.23948 91484 14093 91664 14728 722 x 10^{70}	-3.55109 59039 00731 77995 57258 289 x 10^{72}	-4.20918 33669 92515 24030 37021 756 x 10^{72}

pushed higher to $N=38$ for (1,0,0), $N=67$ for (0,0,1), and $N=112$ for (0,1,0). For (1,0,0) the alternating-sign contribution is moderately larger than for the ground state—a consequence of the increased value of n_1. For (0,0,1) and (0,1,0), the alternating-sign contribution is significantly smaller, which is a consequence of the dependence on n_2 and m that bring it down from the same-sign contribution by a factor of N^{-8n_2-4m-5}. Thus, for (0,1,0) the alternating-sign contribution is $\sim -10^{-25}$ versus $\sim -10^{-10}$ for the ground state.

Comparison of Table X with Table IV reveals clearly that the $\beta_1^{(N)}$ becomes asymptotic much more slowly than the $\beta_2^{(N)}$.

TABLE IX. Coefficients $A(n_1,n_2,m)$, $B(n_1,n_2,m)$, $C(n_1,n_2,m)$, and $D(n_1,n_2,m)$ for the alternating-sign contributions to the asymptotics of $\beta_1^{(N)}$, as in Eq. (232), and to the asymptotics of $E^{(N)}$, as in Eq. (236).

n_1	n_2	m	$A(n_1,n_2,m)$	$B(n_1,n_2,m)$	$C(n_1,n_2,m)$	$D(n_1,n_2,m)$
0	0	0	83	-120	243	-184
1	0	0	2983	-2656	6179	-3680
0	1	0	7459/9	-4960/3	22039/9	-7264/3
0	0	1	2060	-6848/3	13492/3	-9536/3

X. NUMERICAL CHARACTERIZATION OF THE ENERGY SERIES

The asymptotics of the RSPT coefficients $E^{(N)}$ for the energy are similar to those for the $\beta_1^{(N)}$: again there is an alternating-sign contribution down several powers of N from the dominant same-sign contribution [cf. Eq. (199)]. First we list in Tables XI–XIV the terms of the RSPT series, the exponentially small gap series $\Delta E^{\{1\}}$, and the doubly-exponentially-small imaginary series $\Delta_i E^{\{2\}}$, all through fifty-first order in $(2R/n)^{-1}$, for the ground state $(n_1=n_2=m=0)$ and for the three $n=2$ excited states for which n_1, n_2, and m are (1,0,0), and (0,1,0) and (0,0,1). We use the notation $C^{\{1\}(N)}$ and $C^{\{2\}(N)}$ for the series coefficients for the two exponentially small quantities, according to [cf. Eqs. (176) and (179)]

$$\Delta E^{\{1\}} = \pm \frac{(2R/n)^{2\beta_2^{(0)}} e^{-R/n-n}}{n^3 n_2!(n_2+m)!} \sum_{N=0}^{\infty} C^{\{1\}(N)}(2R/n)^{-N} , \tag{234}$$

$$\Delta_i E^{\{2\}} = \mp \pi \frac{(2R/n)^{4\beta_2^{(0)}} e^{-2R/n-2n}}{n^3[n_2!(n_2+m)!]^2} \times \sum_{N=0}^{\infty} C^{\{2\}(N)}(2R/n)^{-N} \quad (\pm \mathrm{Im} R \geq 0) . \tag{235}$$

As for β_1 and β_2, the coefficients are estimated to be accurate to the precision reported [29 digits for $(n_1,n_2,m)=(0,0,0)$, (1,0,0), and (0,0,1), and 27 digits for (0,1,0)]. We call the reader's attention to the sign pattern, which settles down quickly to uniform minus signs for the ground state and two of the excited states, but which is quite irregular until after twenty-seventh order for the (1,0,0) state.

The asymptotics of the $E^{(N)}$ have two contributions, as did the $\beta_1^{(N)}$. In the notation of Eq. (235), Eq. (199) becomes

$$\begin{aligned} E^{(N)} \sim & -\frac{e^{-2n}(N+4n_2+2m+1)!}{n^3(n_2!)^2[(n_2+m)!]^2}\left[1+\frac{C^{\{2\}(1)}}{N+4n_2+2m+1}+\frac{C^{\{2\}(2)}}{(N+4n_2+2m+1)(N+4n_2+2m)}+\cdots\right] \\ & +(-1)^{m+N-1}e^{2n}16n\frac{(n_1+2n_2+2m+1)!(n_1+2n_2+m+1)!}{n_1!(n_1+m)!}(N-4n_2-2m-5)! \\ & \times\left[1+\frac{12n^2-12(\beta_2^{(0)})^2+m^2-1+12n-12\beta_2^{(0)}-4n\beta_2^{(0)}}{N-4n_2-2m-5}\right. \\ & -\frac{4n^2[2\psi(N-4n_2-2m-5)-\psi(n_1+2n_2+2m+2)-\psi(n_1+2n_2+m+2)]}{N-4n_2-2m-5} \\ & +\frac{C(n_1,n_2,m)+8\pi^2n^4/3+D(n_1,n_2,m)[\psi(N-4n_2-2m-6)-\psi(1)]}{(N-4n_2-2m-5)(N-4n_2-2m-6)} \\ & \left.+32n^4\frac{[\psi(N-4n_2-2m-6)-\psi(1)]^2+[\psi^{(1)}(N-4n_2-2m-6)-\psi^{(1)}(1)]}{(N-4n_2-2m-5)(N-4n_2-2m-6)}+O(N^{-3}(\ln N)^3)\right] , \end{aligned} \tag{236}$$

where the coefficients $C(n_1,n_2,m)$ and $D(n_1,n_2,m)$ are independent of N. The first few are listed in Table IX.

In Table XV we uncover numerically the alternating-sign contributions to the asymptotics by subtracting the terms in Eq. (236) that come from $\Delta_i E^{\{2\}}$ (those involving the coefficients $C^{\{2\}(k)}$). We truncate the partial sum after including the smallest term. Listed in Table XV are the exact $E^{(N)}$, the k index of the last correction term included in the partial sum and the value of that term, the difference between the exact and asymptotic values—

TABLE X. Asymptotic analysis of the RSPT $\beta_1^{(N)}$. The dominant, same-sign subseries in the asymptotic formula (232) of the text is truncated with the inclusion of the smallest term, whose index has been indicated by $k_{\min}$. The relative asymptotic error refers to the difference between the exact coefficient $\beta_1^{(N)}$ and the asymptotic formula to the indicated number of terms, divided by the leading asymptotic term, which is $(4n_1+2m+2)(N+4n_2+2m)!/(n_2!)^2[(n_2+m)!]^2$. For sufficiently large N, the relative asymptotic error, after accounting for the same-sign subseries, is alternating in sign. The effect of the alternating-sign subseries is seen through the inclusion of up to three terms.

		same-sign subseries			alternating-sign subseries: relative asymptotic error after inclusion of terms through order (in N^{-1})		
N	$\beta_1^{(N)}$(exact)	$k_{\min}$	smallest term	relative asymptotic error	0	1	2
	Ground state: $n_1=0$, $n_2=0$, $m=0$						
30	4.20484 95981 43437 52856 90821 189 $\times 10^{32}$	14	1.1×10^{-6}	-3.6×10^{-7}	1.0×10^{-7}	-2.0×10^{-7}	-1.6×10^{-7}
31	1.31482 83626 14689 16879 39208 591 $\times 10^{34}$	14	5.8×10^{-7}	-2.1×10^{-7}	-6.1×10^{-7}	-3.6×10^{-7}	-3.9×10^{-7}
32	4.24136 03481 22180 14997 27011 495 $\times 10^{35}$	15	3.2×10^{-7}	-2.3×10^{-7}	1.0×10^{-7}	-1.0×10^{-7}	-7.1×10^{-8}
33	1.41014 46206 91339 49621 17275 387 $\times 10^{37}$	15	1.8×10^{-7}	7.0×10^{-9}	-2.7×10^{-7}	-1.0×10^{-7}	-1.3×10^{-7}
34	4.82802 38503 08125 29553 31706 145 $\times 10^{38}$	16	9.5×10^{-8}	-1.5×10^{-7}	9.4×10^{-8}	-5.0×10^{-8}	-2.8×10^{-8}
35	1.70085 93393 95120 27806 01785 581 $\times 10^{40}$	16	5.2×10^{-8}	6.3×10^{-8}	-1.4×10^{-7}	-2.1×10^{-8}	-4.0×10^{-8}
36	6.16061 45090 62291 67417 63524 285 $\times 10^{41}$	17	2.8×10^{-8}	-1.0×10^{-7}	7.7×10^{-8}	-2.6×10^{-8}	-9.8×10^{-9}
37	2.29254 43917 84602 54356 91615 649 $\times 10^{43}$	17	1.5×10^{-8}	6.7×10^{-8}	-8.6×10^{-8}	1.6×10^{-9}	-1.2×10^{-8}
38	8.75883 13712 37131 11125 90672 419 $\times 10^{44}$	18	8.0×10^{-9}	-7.4×10^{-8}	5.9×10^{-8}	-1.5×10^{-8}	-3.3×10^{-9}
39	3.43337 61289 94263 40892 50487 074 $\times 10^{46}$	18	4.3×10^{-9}	5.9×10^{-8}	-5.7×10^{-8}	6.5×10^{-9}	-3.6×10^{-9}
40	1.37996 71455 77679 10787 76135 778 $\times 10^{48}$	19	2.3×10^{-9}	-5.6×10^{-8}	4.5×10^{-8}	-9.7×10^{-9}	-1.0×10^{-9}
45	2.06510 55699 12521 40804 36906 726 $\times 10^{56}$	22	9.6×10^{-11}	3.1×10^{-8}	-2.3×10^{-8}	4.2×10^{-9}	-4.9×10^{-11}
60	1.49440 30280 94080 16957 06185 790 $\times 10^{82}$	29	5.6×10^{-15}	-7.9×10^{-9}	4.3×10^{-9}	-6.9×10^{-10}	2.9×10^{-11}
75	4.55831 63582 14424 59695 34188 535 $\times 10^{109}$	37	2.7×10^{-19}	2.7×10^{-9}	-1.2×10^{-9}	1.7×10^{-10}	-8.2×10^{-12}
90	2.77057 11141 95650 94203 64577 899 $\times 10^{138}$	44	1.2×10^{-23}	-1.1×10^{-9}	4.1×10^{-10}	-5.2×10^{-11}	2.6×10^{-12}
105	2.03771 32634 96922 30359 18117 521 $\times 10^{168}$	51	5.0×10^{-28}	5.2×10^{-10}	-1.7×10^{-10}	1.9×10^{-11}	-9.5×10^{-13}
120	1.27029 42073 70747 46762 41761 449 $\times 10^{199}$	51	6.0×10^{-32}	-2.7×10^{-10}	7.9×10^{-11}	-8.2×10^{-12}	3.9×10^{-13}
135	5.13952 02223 01706 16760 56611 113 $\times 10^{230}$	51	2.9×10^{-35}	1.5×10^{-10}	-4.0×10^{-11}	3.8×10^{-12}	-1.7×10^{-13}
150	1.09657 73249 78189 64805 40729 875 $\times 10^{263}$	51	3.8×10^{-38}	-9.1×10^{-11}	2.2×10^{-11}	-1.9×10^{-12}	8.4×10^{-14}
	Excited state: $n_1=1$, $n_2=0$, $m=0$						
35	4.63527 95548 81703 42107 57979 025 $\times 10^{40}$	21	1.0×10^{-7}	6.0×10^{-6}	1.6×10^{-6}	8.7×10^{-6}	8.5×10^{-6}
36	1.68397 18149 95061 54938 41790 695 $\times 10^{42}$	21	4.2×10^{-8}	1.3×10^{-5}	1.7×10^{-5}	1.1×10^{-5}	1.1×10^{-5}
37	6.28413 68274 68655 29873 69117 033 $\times 10^{43}$	21	1.8×10^{-8}	-3.3×10^{-6}	-6.6×10^{-6}	-1.4×10^{-6}	-1.8×10^{-6}
38	2.40732 62624 95121 58317 30959 517 $\times 10^{45}$	21	8.1×10^{-9}	-8.9×10^{-7}	1.9×10^{-6}	-2.5×10^{-6}	-2.0×10^{-6}
39	9.46037 67189 73453 98270 12646 060 $\times 10^{46}$	21	3.7×10^{-9}	6.9×10^{-7}	-1.8×10^{-6}	2.1×10^{-6}	1.5×10^{-6}
40	3.81149 49519 09701 02495 76615 853 $\times 10^{48}$	21	1.8×10^{-9}	-1.7×10^{-7}	2.0×10^{-6}	-1.3×10^{-6}	-8.3×10^{-7}
41	1.57340 44239 91749 11825 05650 717 $\times 10^{50}$	21	8.6×10^{-10}	9.1×10^{-8}	-1.8×10^{-6}	1.1×10^{-6}	5.9×10^{-7}
42	6.65115 23979 40872 72589 32947 434 $\times 10^{51}$	21	4.3×10^{-10}	-1.2×10^{-7}	1.6×10^{-6}	-9.6×10^{-7}	-5.0×10^{-7}
43	2.87760 16315 26658 55137 53854 547 $\times 10^{53}$	21	2.2×10^{-10}	1.3×10^{-7}	-1.4×10^{-6}	8.4×10^{-7}	4.1×10^{-7}
44	1.27355 17426 99160 79925 99461 395 $\times 10^{55}$	21	1.2×10^{-10}	-1.2×10^{-7}	1.2×10^{-6}	-7.3×10^{-7}	-3.3×10^{-7}
45	5.76288 84684 97828 21323 99269 039 $\times 10^{56}$	21	6.2×10^{-11}	1.1×10^{-7}	-1.1×10^{-6}	6.4×10^{-7}	2.7×10^{-7}
60	4.25469 21649 34195 83172 33508 800 $\times 10^{82}$	29	5.0×10^{-15}	-4.7×10^{-8}	2.1×10^{-7}	-1.1×10^{-7}	-1.4×10^{-8}
75	1.31285 33314 91568 17177 38410 795 $\times 10^{110}$	37	2.5×10^{-19}	2.1×10^{-8}	-6.2×10^{-8}	2.8×10^{-8}	4.4×10^{-10}
90	8.03918 89765 54943 53588 04877 827 $\times 10^{138}$	44	1.1×10^{-23}	-1.0×10^{-8}	2.2×10^{-8}	-9.1×10^{-9}	3.4×10^{-10}
105	5.94338 14608 72294 73269 41028 217 $\times 10^{168}$	51	4.7×10^{-28}	5.3×10^{-9}	-9.4×10^{-9}	3.5×10^{-9}	-2.3×10^{-10}
120	3.71916 15533 21328 05918 28739 902 $\times 10^{199}$	51	5.7×10^{-32}	-3.0×10^{-9}	4.5×10^{-9}	-1.5×10^{-9}	1.2×10^{-10}
135	1.50912 32797 30865 49194 88339 840 $\times 10^{231}$	51	2.7×10^{-35}	1.8×10^{-9}	-2.3×10^{-9}	7.3×10^{-10}	-6.3×10^{-11}
150	3.22727 61757 73613 99640 39047 709 $\times 10^{263}$	51	3.6×10^{-38}	-1.1×10^{-9}	1.3×10^{-9}	-3.8×10^{-10}	3.4×10^{-11}
	Excited state: $n_1=0$, $n_2=1$, $m=0$						
110	3.84066 68154 66344 53494 67272 941 $\times 10^{186}$	51	4.8×10^{-24}	-2.1×10^{-23}	-4.3×10^{-24}	-2.3×10^{-23}	-1.4×10^{-23}
111	4.42831 79529 24774 51625 18522 473 $\times 10^{188}$	51	2.7×10^{-24}	-5.2×10^{-24}	-2.0×10^{-23}	-3.5×10^{-24}	-1.2×10^{-23}
112	5.15003 51797 28241 91850 55330 994 $\times 10^{190}$	51	1.5×10^{-24}	-1.0×10^{-23}	3.4×10^{-24}	-1.1×10^{-23}	-4.3×10^{-24}
113	6.04072 59073 33858 38876 59420 723 $\times 10^{192}$	51	8.4×10^{-25}	1.8×10^{-25}	-1.2×10^{-23}	1.4×10^{-24}	-5.0×10^{-24}
114	7.14569 41846 99620 35747 03243 307 $\times 10^{194}$	51	4.8×10^{-25}	-5.4×10^{-24}	5.2×10^{-24}	-6.4×10^{-24}	-8.1×10^{-25}
115	8.52403 88989 87193 37750 23460 236 $\times 10^{196}$	51	2.7×10^{-25}	1.8×10^{-24}	-7.7×10^{-24}	2.6×10^{-24}	-2.3×10^{-24}
116	1.02532 59914 08535 71897 61735 152 $\times 10^{199}$	51	1.6×10^{-25}	-3.4×10^{-24}	5.0×10^{-24}	-4.1×10^{-24}	2.6×10^{-25}
117	1.24355 32652 55245 94115 13581 471 $\times 10^{201}$	51	9.0×10^{-26}	2.0×10^{-24}	-5.5×10^{-24}	2.5×10^{-24}	-1.3×10^{-24}
118	1.52062 98594 46173 47627 08109 775 $\times 10^{203}$	51	5.3×10^{-26}	-2.4×10^{-24}	4.3×10^{-24}	-2.8×10^{-24}	5.1×10^{-25}

TABLE X. (*Continued*).

		same-sign subseries			alternating-sign subseries		
				relative	relative asymptotic error after inclusion of terms through order (in N^{-1})		
			smallest	asymptotic			
N	$\beta_1^{(N)}$(exact)	k_{min}	term	error	0	1	2
119	$1.87460\,86416\,42265\,94460\,30816\,980 \times 10^{205}$	51	3.1×10^{-26}	1.8×10^{-24}	-4.2×10^{-24}	2.2×10^{-24}	-8.1×10^{-25}
120	$2.32968\,62305\,67245\,00079\,98391\,415 \times 10^{207}$	51	1.8×10^{-26}	-1.9×10^{-24}	3.5×10^{-24}	-2.1×10^{-24}	5.0×10^{-25}
125	$7.77622\,45330\,15126\,32981\,58236\,992 \times 10^{217}$	51	1.4×10^{-27}	1.1×10^{-24}	-2.1×10^{-24}	1.1×10^{-24}	-3.2×10^{-25}
130	$3.14585\,46826\,64292\,16242\,59039\,798 \times 10^{228}$	51	1.2×10^{-28}	-6.6×10^{-25}	1.2×10^{-24}	-6.3×10^{-25}	1.7×10^{-25}
135	$1.53154\,39326\,78469\,42414\,90862\,477 \times 10^{239}$	51	1.2×10^{-29}	4.2×10^{-25}	-7.2×10^{-25}	3.7×10^{-25}	-9.7×10^{-26}
140	$8.91417\,76528\,46513\,18858\,83709\,809 \times 10^{249}$	51	1.3×10^{-30}	-2.7×10^{-25}	4.4×10^{-25}	-2.2×10^{-25}	5.6×10^{-26}
145	$6.16495\,21436\,76917\,94321\,95285\,938 \times 10^{260}$	51	1.5×10^{-31}	1.7×10^{-25}	-2.7×10^{-25}	1.3×10^{-25}	-3.3×10^{-26}
150	$5.03716\,89616\,45249\,73328\,18252\,223 \times 10^{271}$	51	2.0×10^{-32}	-1.1×10^{-25}	1.7×10^{-25}	-7.9×10^{-26}	2.0×10^{-26}
	Excited state: $n_1=0$, $n_2=0$, $m=1$						
65	$1.13885\,00590\,21654\,30449\,69843\,011 \times 10^{95}$	31	3.3×10^{-14}	-4.2×10^{-14}	7.3×10^{-15}	-6.0×10^{-14}	-3.0×10^{-14}
66	$7.77531\,43019\,45827\,29475\,89791\,639 \times 10^{96}$	32	1.7×10^{-14}	-1.0×10^{-15}	-4.4×10^{-14}	1.4×10^{-14}	-1.2×10^{-14}
67	$5.38584\,79493\,22852\,74308\,15564\,229 \times 10^{98}$	32	9.4×10^{-15}	-1.7×10^{-14}	2.0×10^{-14}	-2.9×10^{-14}	-7.3×10^{-15}
68	$3.78430\,66855\,26025\,29819\,08827\,997 \times 10^{100}$	33	5.0×10^{-15}	3.7×10^{-15}	-2.9×10^{-14}	1.4×10^{-14}	-4.9×10^{-15}
69	$2.69667\,40945\,68716\,52063\,62962\,081 \times 10^{102}$	33	2.7×10^{-15}	-8.6×10^{-15}	2.0×10^{-14}	-1.7×10^{-14}	-9.4×10^{-16}
70	$1.94848\,30612\,01337\,28345\,91680\,476 \times 10^{104}$	34	1.4×10^{-15}	4.3×10^{-15}	-2.1×10^{-14}	1.2×10^{-14}	-2.5×10^{-15}
71	$1.42728\,01030\,14265\,96995\,99307\,339 \times 10^{106}$	34	7.6×10^{-16}	-5.5×10^{-15}	1.6×10^{-14}	-1.2×10^{-14}	6.5×10^{-16}
72	$1.05970\,92346\,33030\,19251\,82579\,320 \times 10^{108}$	35	4.0×10^{-16}	3.9×10^{-15}	-1.5×10^{-14}	9.0×10^{-15}	-1.5×10^{-15}
73	$7.97355\,05617\,87022\,18242\,21594\,741 \times 10^{109}$	35	2.2×10^{-16}	-4.0×10^{-15}	1.3×10^{-14}	-8.3×10^{-15}	9.0×10^{-16}
74	$6.07895\,46016\,11356\,16506\,76649\,181 \times 10^{111}$	36	1.1×10^{-16}	3.3×10^{-15}	-1.2×10^{-14}	6.9×10^{-15}	-1.1×10^{-15}
75	$4.69509\,80519\,05535\,03298\,01084\,668 \times 10^{113}$	36	6.1×10^{-17}	-3.1×10^{-15}	1.0×10^{-14}	-6.1×10^{-15}	8.2×10^{-16}
90	$4.17505\,47693\,53232\,78059\,13419\,611 \times 10^{142}$	44	4.1×10^{-21}	7.0×10^{-16}	-1.7×10^{-15}	9.1×10^{-16}	-1.5×10^{-16}
105	$4.22596\,42190\,25580\,41268\,06350\,781 \times 10^{172}$	51	2.4×10^{-25}	-2.0×10^{-16}	3.9×10^{-16}	-1.8×10^{-16}	3.1×10^{-17}
120	$3.46896\,63375\,28781\,08724\,93612\,405 \times 10^{203}$	51	3.6×10^{-29}	6.5×10^{-17}	-1.1×10^{-16}	4.6×10^{-17}	-7.6×10^{-18}
135	$1.78742\,61945\,40356\,87670\,07584\,213 \times 10^{235}$	51	2.0×10^{-32}	-2.4×10^{-17}	3.5×10^{-17}	-1.3×10^{-17}	2.2×10^{-18}
150	$4.73149\,48064\,78678\,81088\,48155\,313 \times 10^{267}$	51	3.0×10^{-35}	1.0×10^{-17}	-1.3×10^{-17}	4.5×10^{-18}	-7.0×10^{-19}

divided by the leading asymptotic term (called the relative asymptotic error in the table), and the relative asymptotic error after taking account of one, two, and three terms from the alternating-sign asymptotic formula. These quantities are listed for various orders, up to order 150.

Notice that for the ground state the residual remaining after subtraction of the same-sign terms is alternating in sign after order $N=25$, and that it has relative magnitude 7×10^{-11} at order 150—which is small compared to unity, but large compared with the corresponding relative residual for $\beta_2^{(N)}$, which at order 110 is already less than 10^{-30}. The first alternating-sign asymptotic contribution significantly overcompensates, but by the third alternating-sign contribution the relative error has dropped by a factor of 10^{-4} at $N=150$ (see Table XV).

For the excited states, the threshold for alternation is pushed higher to $N=39$ for (1,0,0), $N=50$ for (0,0,1), and $N=93$ for (0,1,0). For (1,0,0) the alternating-sign contribution is significantly larger than for the ground state—a consequence of the increased value of n_1. For (0,0,1) and (0,1,0), the alternating-sign contribution is significantly smaller, which is a consequence of the dependence on n_2 and m that brings it down from the same-sign contribution by a factor of N^{-8n_2-4m-6}. Thus, for (0,1,0) the alternating-sign contribution is $\sim 5\times 10^{-24}$, versus $\sim 7\times 10^{-11}$ for the ground state.

Comparison of Table XV with Tables IV and X reveals clearly that like the $\beta_1^{(N)}$, the $E^{(N)}$ become asymptotic much more slowly than the $\beta_2^{(N)}$.

It is of some interest to turn to an observation made in Ref. 13, that the "Neville table" for the ground-state $E^{(N)}$ seems to converge in a zigzag fashion,[12] and that much better convergence is obtained by treating the even and odd terms separately. An aim of that study was to confirm the asymptotic behavior, $E^{(N)} \sim -e^{-2n}(N+1)!$. The Neville table for the quantities a_N is the matrix, defined recursively with $a_N^0 = a_N$,

$$a_N^k = [N a_N^{k-1} - (N-k) a_{N-1}^{k-1}]/k \; . \tag{237}$$

If a_N is given asymptotically by the expression

$$a_N \sim 1 + A/N + B/[N(N-1)] + C/[N(N-1)(N-2)] + \cdots \; , \tag{238}$$

then the difference between each entry and unity, $a_N^k - 1$, approaches 0 as N^{-k-1}. If, however, a_N has additional terms, say of the form

$$(-1)^N D/[N(N-1)(N-2)(N-3)(N-4)(N-5)] \; ,$$

as is the case for $E^{(N)}$ for the ground state, then the entry a_N^k has an alternating-sign contribution proportional to N^{k-6}. That is, the difference with unity has an alternating-sign contribution that *grows* with k. This is the explanation of alternation phenomenon observed in Ref. 13. If the alternating-sign contribution could be eliminated, then the Neville table should converge more

TABLE XI. Coefficients for the RSPT series, the $\Delta E^{(1)}$ series, and the $\Delta_i E^{(2)}$ series, as defined by Eqs. (166), (234), and (235) of the text, for the ($n_1=0$, $n_2=0$, $m=0$) ground state of H_2^+.

Order N	Coefficient $E^{(N)}$	$C^{(1)(N)}$	$C^{(2)(N)}$
0	-5.00000 00000 00000 00000 00000 000 x 10^{-1}	1.00000 00000 00000 00000 00000 000 x 10^{0}	1.00000 00000 00000 00000 00000 000 x 10^{0}
1	-2.00300 00000 00000 00000 00000 000 x 10^{0}	1.00000 00000 00000 00000 00000 000 x 10^{0}	2.00000 00000 00000 00000 00000 000 x 10^{0}
2	0.00000 00000 00000 00000 00000 000 x 10^{0}	-1.25000 00000 00000 00000 00000 000 x 10^{1}	-1.80000 00000 00000 00000 00000 000 x 10^{1}
3	0.00000 00000 00000 00000 00000 000 x 10^{0}	-2.18333 33333 33333 33333 33333 333 x 10^{1}	-6.46666 66666 66666 66666 66666 667 x 10^{1}
4	-3.60000 00000 00000 00000 00000 000 x 10^{1}	-1.63458 33333 33333 33333 33333 333 x 10^{2}	-1.40333 33333 33333 33333 33333 333 x 10^{2}
5	0.00000 00000 00000 00000 00000 000 x 10^{0}	-1.21165 83333 33333 33333 33333 333 x 10^{3}	-1.52440 00000 00000 00000 00000 000 x 10^{3}
6	-4.80000 00000 00000 00000 00000 000 x 10^{2}	-7.24887 36111 11111 11111 11111 111 x 10^{3}	-1.24825 77777 77777 77777 77777 778 x 10^{4}
7	-6.81600 00000 00000 00000 00000 000 x 10^{3}	-1.01012 48313 49206 34920 63492 063 x 10^{5}	-1.24665 30793 65079 36507 93650 794 x 10^{5}
8	-3.10200 00000 00000 00000 00000 000 x 10^{4}	-9.36248 50969 74206 34920 63492 063 x 10^{5}	-1.32387 27047 61904 76190 47619 048 x 10^{6}
9	-4.53888 00000 00000 00000 00000 000 x 10^{5}	-1.03330 47428 96549 82363 31569 665 x 10^{7}	-1.48066 78106 52557 31922 39858 907 x 10^{7}
10	-5.42457 60000 00000 00000 00000 000 x 10^{6}	-1.39652 81569 23856 37125 22045 855 x 10^{8}	-1.90613 92758 70194 00352 73368 607 x 10^{8}
11	-5.95039 68000 00000 00000 00000 000 x 10^{7}	-1.78848 65467 99068 53755 81208 915 x 10^{9}	-2.52087 44293 93246 75324 67532 468 x 10^{9}
12	-8.38205 20800 00000 00000 00000 000 x 10^{8}	-2.56750 96449 21180 08687 23611 779 x 10^{10}	-3.59704 02597 82538 82742 77163 166 x 10^{10}
13	-1.18278 18240 00000 00000 00000 000 x 10^{10}	-3.93101 33620 54025 84926 48683 621 x 10^{11}	-5.49379 21993 59230 00127 44457 189 x 10^{11}
14	-1.78418 03616 00000 00000 00000 000 x 10^{11}	-6.30860 30120 96369 94706 69711 865 x 10^{12}	-8.84328 05607 80952 19263 98116 874 x 10^{12}
15	-2.89561 86272 64000 00000 00000 000 x 10^{12}	-1.07905 21375 52958 94081 47697 134 x 10^{14}	-1.51035 49002 20563 37248 24107 893 x 10^{14}
16	-4.94927 77000 42800 00000 00000 000 x 10^{13}	-1.94504 09431 65771 57196 65044 203 x 10^{15}	-2.72136 22449 18935 43643 79387 025 x 10^{15}
17	-8.95386 41889 94560 00000 00000 000 x 10^{14}	-3.69190 69424 98668 33380 88003 127 x 10^{16}	-5.16228 40287 16972 74018 42068 987 x 10^{16}
18	-1.70775 91118 31129 60000 00000 000 x 10^{16}	-7.36691 08866 93962 34950 04035 051 x 10^{17}	-1.02917 32010 86507 40966 31176 246 x 10^{18}
19	-3.42401 84054 44785 60000 00000 000 x 10^{17}	-1.54150 20632 41004 58513 97150 697 x 10^{19}	-2.15160 26728 99255 60149 59473 763 x 10^{19}
20	-7.20352 71847 96734 02400 00000 000 x 10^{18}	-3.37647 18615 98035 45095 74336 884 x 10^{20}	-4.70830 56141 97598 24827 92116 495 x 10^{20}
21	-1.58663 37018 30904 41984 00000 000 x 10^{20}	-7.72759 80864 27204 89987 64471 393 x 10^{21}	-1.07651 94098 84186 93990 97946 024 x 10^{22}
22	-3.65198 45724 20448 69676 80000 000 x 10^{21}	-1.84481 55054 45899 90504 36842 115 x 10^{23}	-2.56744 52149 71371 40328 15826 700 x 10^{23}
23	-8.76818 18011 54661 46806 40000 000 x 10^{22}	-4.58661 97503 05278 22926 67251 432 x 10^{24}	-6.37699 28377 52626 56173 21947 749 x 10^{24}
24	-2.19237 89692 87299 63470 43120 000 x 10^{24}	-1.18581 57747 76732 14364 04939 318 x 10^{26}	-1.64709 96320 07583 72117 51034 632 x 10^{26}
25	-5.69988 90347 32373 98500 94080 000 x 10^{25}	-3.18355 83644 61635 78147 16798 644 x 10^{27}	-4.41778 93549 93934 37636 08871 324 x 10^{27}
26	-1.53868 45406 24901 90391 24834 560 x 10^{27}	-8.86359 51548 82034 55518 28981 017 x 10^{28}	-1.22885 62062 29670 07480 29362 914 x 10^{29}
27	-4.30701 59428 07344 63159 84849 344 x 10^{28}	-2.55604 56435 44030 79195 81850 995 x 10^{30}	-3.54055 42239 64881 51860 39522 499 x 10^{30}
28	-1.24856 46387 44255 27154 90329 645 x 10^{30}	-7.62581 42566 49438 26356 68133 888 x 10^{31}	-1.05538 73385 15058 26984 64609 363 x 10^{32}
29	-3.74403 87313 41340 10875 15630 039 x 10^{31}	-2.35118 32175 44112 98058 07830 405 x 10^{33}	-3.25123 45534 80517 31436 45408 326 x 10^{33}
30	-1.16009 28518 92770 55962 92709 845 x 10^{33}	-7.48383 74003 70202 63362 29847 182 x 10^{34}	-1.03403 30618 00998 71361 63200 561 x 10^{35}
31	-3.71037 69005 48712 87703 51920 613 x 10^{34}	-2.45684 57197 25637 52075 09725 748 x 10^{36}	-3.39194 73866 39399 86362 25343 054 x 10^{36}
32	-1.22376 73764 98047 98279 36551 621 x 10^{36}	-8.31096 43578 93358 83865 73372 462 x 10^{37}	-1.14655 69540 07235 99096 60792 257 x 10^{38}
33	-4.15850 46386 52791 79250 06421 463 x 10^{37}	-2.89447 16053 73106 19866 75975 367 x 10^{39}	-3.99023 68870 75134 01710 49666 266 x 10^{39}
34	-1.45466 05269 16266 44223 27876 155 x 10^{39}	-1.03699 81564 05009 79484 75183 657 x 10^{41}	-1.42857 74193 90117 87840 82240 525 x 10^{41}
35	-5.23380 98909 58899 15495 95876 552 x 10^{40}	-3.81892 67651 11900 66517 64777 557 x 10^{42}	-5.25744 62109 52309 55992 57531 415 x 10^{42}
36	-1.93541 35686 18694 56546 97666 524 x 10^{42}	-1.44458 10606 36116 14398 05282 839 x 10^{44}	-1.98743 80445 14512 84289 85592 760 x 10^{44}
37	-7.35041 52418 21237 84191 62047 088 x 10^{43}	-5.60889 61415 57971 74124 95354 039 x 10^{45}	-7.71183 32271 33780 24422 34967 571 x 10^{45}
38	-2.86505 73217 61526 57741 39553 536 x 10^{45}	-2.23388 80962 10866 74370 87630 041 x 10^{47}	-3.06958 62026 56960 89416 43834 872 x 10^{47}
39	-1.14538 73358 92800 41315 04907 402 x 10^{47}	-9.12054 35207 82225 47645 27322 087 x 10^{48}	-1.25252 61489 84422 94865 32767 287 x 10^{49}
40	-4.69352 18341 43224 86001 66161 484 x 10^{48}	-3.81501 09910 40204 37163 01749 417 x 10^{50}	-5.23622 58322 48921 38716 29520 814 x 10^{50}
41	-1.97021 71451 55716 54651 93292 483 x 10^{50}	-1.63394 92914 80080 03879 36472 874 x 10^{52}	-2.24143 56144 80234 39000 70866 983 x 10^{52}
42	-8.46745 17579 34230 37130 94628 568 x 10^{51}	-7.16164 61078 88398 19543 79712 967 x 10^{53}	-9.81914 64503 04750 45017 14147 510 x 10^{53}
43	-3.72374 19906 83640 20995 29606 338 x 10^{53}	-3.21064 65125 22034 10147 66875 402 x 10^{55}	-4.39981 49010 52360 91191 82712 265 x 10^{55}
44	-1.67483 04120 56231 51325 53616 379 x 10^{55}	-1.47150 46629 92978 43009 77197 609 x 10^{57}	-2.01554 24510 55075 37912 12031 149 x 10^{57}
45	-7.70037 25595 40304 33979 57208 022 x 10^{56}	-6.89149 31471 87806 72268 13012 454 x 10^{58}	-9.43494 05210 86612 28038 44183 269 x 10^{58}
46	-3.61740 69023 44197 63149 03727 041 x 10^{58}	-3.29647 34909 93636 44250 90128 325 x 10^{60}	-4.51105 03260 68594 13184 53084 808 x 10^{60}
47	-1.73552 47980 40244 27895 64957 019 x 10^{60}	-1.60983 10532 42913 94475 07304 622 x 10^{62}	-2.20199 90640 66198 93151 05453 051 x 10^{62}
48	-8.50009 57733 00430 30156 86665 842 x 10^{61}	-8.02275 02931 69226 37180 63385 367 x 10^{63}	-1.09692 00611 48850 99681 67460 533 x 10^{64}
49	-4.24810 45332 68548 46607 67018 480 x 10^{63}	-4.07852 65026 06111 74618 73019 639 x 10^{65}	-5.57411 32964 57813 71075 94343 361 x 10^{65}
50	-2.16556 55778 20181 55845 44248 962 x 10^{65}	-2.11422 94904 67728 48102 87477 156 x 10^{67}	-2.88835 80523 22927 76072 66918 834 x 10^{67}
51	-1.12560 24353 67844 96777 46394 055 x 10^{67}	-1.11714 04828 30431 70236 36058 355 x 10^{69}	-1.52559 23473 13970 04827 93441 687 x 10^{69}

normally. In Table XVI we have calculated the Neville table for the quantity $-1-E^{(N)}e^2/(N+1)!$ with up to three alternating-sign contributions removed, as indicated by Eq. (236) and by Table XV. The value before any processing differs from 0 by ~ 0.012 for N between 145 and 150. The subtraction of the alternating-sign terms shows up only in the twelfth decimal place. As the Neville iteration is carried out, the entries without removal of the alternating-sign contribution reach -0.00002 for $k=2$, but then grow to ± 0.024 at $k=4$. The sign alternation is clearly evident. As the leading, $1/N$, and $1/N^2$ alternating-sign terms are incorporated, the growing, alternating-sign behavior is pushed to higher values of k, and the approach of the entries to zero is closer. The best

TABLE XII. Coefficients for the RSPT series, the $\Delta E^{(1)}$ series, and the $\Delta_i E^{(2)}$ series, as defined by Eqs. (166), (234), and (235) of the text, for the $(n_1,n_2,m)=(1,0,0)$ excited state of H_2^+.

Order N	Coefficient $E^{(N)}$	$C^{(1)(N)}$	$C^{(2)(N)}$
0	-1. 25000 00000 00000 00000 00000 000 x 10^{-1}	1. 00000 00000 00000 00000 00000 000 x 10^{0}	1. 00000 00000 00000 00000 00000 000 x 10^{0}
1	-1. 00000 00000 00000 00000 00000 000 x 10^{0}	1. 20000 00000 00000 00000 00000 000 x 10^{1}	2. 40000 00000 00000 00000 00000 000 x 10^{1}
2	3. 00000 00000 00000 00000 00000 000 x 10^{0}	-1. 70000 00000 00000 00000 00000 000 x 10^{1}	1. 22000 00000 00000 00000 00000 000 x 10^{2}
3	-6. 00000 00000 00000 00000 00000 000 x 10^{0}	-2. 69333 33333 33333 33333 33333 333 x 10^{2}	-8. 66666 66666 66666 66666 66666 667 x 10^{2}
4	-7. 80000 00000 00000 00000 00000 000 x 10^{1}	9. 10000 00000 00000 00000 00000 000 x 10^{2}	-4. 47500 00000 00000 00000 00000 000 x 10^{3}
5	1. 22400 00000 00000 00000 00000 000 x 10^{3}	-7. 45733 33333 33333 33333 33333 333 x 10^{3}	3. 19546 66666 66666 66666 66666 667 x 10^{4}
6	-8. 81400 00000 00000 00000 00000 000 x 10^{3}	5. 87785 55555 55555 55555 55555 556 x 10^{4}	-1. 28683 77777 77777 77777 77777 778 x 10^{5}
7	-5. 28000 00000 00000 00000 00000 000 x 10^{2}	-7. 06415 42857 14285 71428 57142 857 x 10^{5}	-9. 87438 85714 28571 42857 14285 714 x 10^{5}
8	8. 27436 00000 00000 00000 00000 000 x 10^{5}	-3. 53690 35873 01587 30158 73015 873 x 10^{6}	9. 95790 05396 82539 68253 96825 397 x 10^{6}
9	-9. 61396 80000 00000 00000 00000 000 x 10^{6}	1. 88686 32944 62081 12874 77954 145 x 10^{8}	-8. 46073 03731 92239 85890 65255 732 x 10^{7}
10	9. 90721 80000 00000 00000 00000 000 x 10^{6}	-3. 15201 17618 01058 20105 82010 582 x 10^{9}	-2. 39704 42908 35978 83597 88359 788 x 10^{8}
11	1. 27262 10240 00000 00000 00000 000 x 10^{9}	1. 28815 59385 49584 73625 14029 181 x 10^{10}	-3. 21851 07104 84143 01747 63508 097 x 10^{9}
12	-1. 99901 00364 00000 00000 00000 000 x 10^{10}	3. 81023 29566 40769 17321 36176 581 x 10^{11}	4. 33491 10283 20819 83859 76163 754 x 10^{10}
13	8. 53720 25136 00000 00000 00000 000 x 10^{10}	-1. 02389 55657 81621 55671 48900 482 x 10^{13}	-1. 18715 17415 68802 85146 95181 362 x 10^{12}
14	2. 15315 34951 24000 00000 00000 000 x 10^{12}	9. 35632 83452 95452 46611 11962 699 x 10^{13}	-2. 39992 56892 79449 59790 35661 575 x 10^{13}
15	-5. 08411 86927 84000 00000 00000 000 x 10^{13}	3. 85854 62758 17243 37551 53331 873 x 10^{14}	5. 13239 50387 76683 74741 22976 769 x 10^{14}
16	4. 36975 77689 27280 00000 00000 000 x 10^{14}	-3. 02931 91770 33217 82359 46064 517 x 10^{16}	-9. 76182 13860 45106 44710 13994 823 x 10^{15}
17	2. 27309 65366 68000 00000 00000 000 x 10^{15}	4. 48498 24456 60625 75432 48386 523 x 10^{17}	-2. 88337 84590 36878 21022 37981 727 x 10^{16}
18	-1. 29108 99772 26249 42000 00000 000 x 10^{17}	-2. 45880 27158 17418 87215 87083 116 x 10^{18}	1. 49556 21500 83097 01324 88019 635 x 10^{18}
19	1. 84814 58775 64340 67200 00000 000 x 10^{18}	-6. 79303 43668 58330 24709 04376 503 x 10^{19}	-5. 34675 75848 58079 53131 26858 617 x 10^{19}
20	-8. 33084 55869 39679 03600 00000 000 x 10^{18}	1. 64252 01268 70773 53086 99674 202 x 10^{21}	1. 54633 15097 94322 94457 05069 356 x 10^{20}
21	-2. 40972 22867 09166 75664 00000 000 x 10^{20}	-2. 30112 63946 06663 17965 20081 224 x 10^{22}	-2. 21360 52023 96051 22924 27711 883 x 10^{21}
22	6. 09101 69950 00482 14223 60000 000 x 10^{21}	-3. 61230 75819 53202 55256 21975 926 x 10^{22}	-2. 50584 90664 58102 43373 17750 518 x 10^{23}
23	-7. 51468 51164 92636 15363 51999 999 x 10^{22}	3. 11833 11862 12830 99609 67381 608 x 10^{24}	-1. 27088 63506 42950 81661 03911 680 x 10^{23}
24	4. 45799 85403 42591 05397 19999 958 x 10^{22}	-1. 26184 17602 52519 49054 53520 383 x 10^{26}	-7. 86996 73272 15504 21484 38953 706 x 10^{25}
25	1. 08630 12941 49210 00574 99680 001 x 10^{25}	1. 59628 06441 87831 60637 72599 200 x 10^{26}	-1. 77906 31207 18445 75737 46227 773 x 10^{27}
26	-3. 32113 46075 60316 24709 48791 604 x 10^{26}	-2. 11549 86193 83311 04688 88562 507 x 10^{28}	-3. 41218 37700 54843 32830 92946 730 x 10^{28}
27	1. 72292 23997 49134 89775 87364 494 x 10^{27}	-8. 42246 28381 03414 45635 40509 730 x 10^{29}	-1. 28293 06078 42347 05692 44169 678 x 10^{30}
28	-4. 47414 20271 47563 05334 34104 099 x 10^{28}	-1. 30087 98641 10446 15623 68850 491 x 10^{31}	-3. 23806 09854 04302 80546 18391 779 x 10^{31}
29	-1. 65861 15772 76205 08915 50927 847 x 10^{30}	-5. 76696 90788 60371 45436 01386 740 x 10^{32}	-9. 75845 26387 98611 17263 25821 676 x 10^{32}
30	-2. 37954 29016 54278 26085 66449 166 x 10^{31}	-1. 63152 67399 37452 08595 28386 649 x 10^{34}	-3. 05362 99087 36676 43129 29934 883 x 10^{34}
31	-1. 24203 33874 78179 98081 22666 394 x 10^{33}	-5. 13239 85663 09207 13998 97200 639 x 10^{35}	-9. 50983 21985 28737 47424 02797 366 x 10^{35}
32	-3. 54702 67825 83947 44775 29012 452 x 10^{34}	-1. 74041 46349 26595 87684 77324 874 x 10^{37}	-3. 13135 11053 71890 51165 18470 806 x 10^{37}
33	-1. 19516 26701 97816 94921 46572 314 x 10^{36}	-5. 82804 60599 29608 17651 08755 412 x 10^{38}	-1. 05487 39712 70658 60728 28247 671 x 10^{39}
34	-4. 20663 29269 84478 44058 81886 028 x 10^{37}	-2. 04721 13913 99884 96056 03412 083 x 10^{40}	-3. 66268 39010 04406 38687 52165 380 x 10^{40}
35	-1. 47781 93269 22509 49398 00218 784 x 10^{39}	-7. 37127 62923 91937 06836 07554 473 x 10^{41}	-1. 31039 00757 92959 77590 48194 142 x 10^{42}
36	-5. 42131 69465 84306 30428 52084 376 x 10^{40}	-2. 72736 36101 25607 79065 29713 533 x 10^{43}	-4. 81861 79188 01250 01683 92780 839 x 10^{43}
37	-2. 03461 96166 09154 99124 05276 702 x 10^{42}	-1. 03759 29809 16116 20193 70873 781 x 10^{45}	-1. 82134 02107 12747 30857 16204 662 x 10^{45}
38	-7. 84562 80622 84487 21909 84822 569 x 10^{43}	-4. 05122 30560 32525 69842 30735 332 x 10^{46}	-7. 06944 68583 01165 03503 25827 492 x 10^{46}
39	-3. 10431 97519 61902 94805 38840 486 x 10^{45}	-1. 62295 45793 49161 02695 75880 397 x 10^{48}	-2. 81590 12538 76096 09805 21502 918 x 10^{48}
40	-1. 25968 87575 41054 10432 57093 241 x 10^{47}	-6. 66601 12631 84854 79432 97128 839 x 10^{49}	-1. 15025 19028 17681 37812 77845 181 x 10^{50}
41	-5. 23747 50130 94393 89530 20851 158 x 10^{48}	-2. 80547 29821 42826 69650 76335 332 x 10^{51}	-4. 81558 78661 67003 15007 25500 657 x 10^{51}
42	-2. 23079 43468 42744 90353 52610 975 x 10^{50}	-1. 20910 84668 99724 79837 60817 927 x 10^{53}	-2. 06496 74807 37093 29418 99378 545 x 10^{53}
43	-9. 72417 45894 88816 20660 32201 663 x 10^{51}	-5. 33344 61157 47437 50139 25217 718 x 10^{54}	-9. 06461 11197 43912 67668 82211 735 x 10^{54}
44	-4. 33750 12238 23479 90153 12750 852 x 10^{53}	-2. 40656 13515 99441 81091 85731 154 x 10^{56}	-4. 07107 88631 34689 63643 31718 159 x 10^{56}
45	-1. 97804 24293 56898 01864 26922 166 x 10^{55}	-1. 11023 50140 03369 15709 91292 612 x 10^{58}	-1. 86972 93001 39003 25397 19637 015 x 10^{58}
46	-9. 22105 32631 10449 88955 27997 887 x 10^{56}	-5. 23417 74637 67647 53852 96920 033 x 10^{59}	-8. 77671 53968 46893 92419 35444 155 x 10^{59}
47	-4. 39063 14994 42184 66619 03868 999 x 10^{58}	-2. 52055 30064 96779 32327 15978 697 x 10^{61}	-4. 20892 76739 67323 48257 10893 164 x 10^{61}
48	-2. 13508 23157 37712 97855 05133 847 x 10^{60}	-1. 23926 39677 92349 83731 44021 570 x 10^{63}	-2. 06106 71076 13584 18954 23307 887 x 10^{63}
49	-1. 05957 13537 85055 12879 30535 346 x 10^{62}	-6. 21820 66425 33572 78929 57093 596 x 10^{64}	-1. 03017 64447 06438 25290 30053 796 x 10^{65}
50	-5. 36552 30971 89024 45500 82759 098 x 10^{63}	-3. 18290 60555 79916 74828 40595 168 x 10^{66}	-5. 25342 34104 40529 75013 18298 572 x 10^{66}
51	-2. 77062 58304 65887 09708 47673 808 x 10^{65}	-1. 66136 75110 70091 61856 23152 256 x 10^{68}	-2. 73222 08689 54459 04897 04853 559 x 10^{68}

example is for $N=150$ and $k=3$, for which the entry with three alternating-sign terms accounted for is 0.000 000 4, and which is an improvement of three orders of magnitude over the corresponding entry with no alternating-sign correction terms.

XI. NUMERICAL SOLUTION FOR β_2 AND SUMMATION OF THE EXPANSIONS

In this section we compare values of β_2 obtained by numerical solution of the eigenvalue equation with values

TABLE XIII. Coefficients for the RSPT series, the $\Delta E^{(1)}$ series, and the $\Delta_i E^{(2)}$ series, as defined by Eqs. (166), (234), and (235) of the text, for the $(n_1,n_2,m)=(0,1,0)$ excited state of $H_2{}^+$.

Order N	Coefficient $E^{(N)}$	$C^{(1)(N)}$	$C^{(2)(N)}$
0	-1. 25000 00000 00000 00000 00000 000 x 10^{-1}	1. 00000 00000 00000 00000 00000 0 x 10^{0}	1. 00000 00000 00000 00000 00000 0 x 10^{0}
1	-1. 00000 00000 00000 00000 00000 000 x 10^{0}	-4. 00000 00000 00000 00000 00000 0 x 10^{0}	-8. 00000 00000 00000 00000 00000 0 x 10^{0}
2	-3. 00000 00000 00000 00000 00000 000 x 10^{0}	-6. 30000 00000 00000 00000 00000 0 x 10^{1}	-7. 40000 00000 00000 00000 00000 0 x 10^{1}
3	-6. 00000 00000 00000 00000 00000 000 x 10^{0}	-2. 77333 33333 33333 33333 33333 3 x 10^{2}	-1. 62666 66666 66666 66666 66666 7 x 10^{2}
4	-9. 00000 00000 00000 00000 00000 000 x 10^{1}	-1. 96766 66666 66666 66666 66666 7 x 10^{3}	3. 88333 33333 33333 33333 33333 3 x 10^{2}
5	-1. 22400 00000 00000 00000 00000 000 x 10^{3}	-3. 08176 00000 00000 00000 00000 0 x 10^{4}	-6. 59786 66666 66666 66666 66666 7 x 10^{3}
6	-1. 19220 00000 00000 00000 00000 000 x 10^{4}	-4. 57557 37777 77777 77777 77777 8 x 10^{5}	-3. 18823 51111 11111 11111 11111 1 x 10^{5}
7	-1. 48464 00000 00000 00000 00000 000 x 10^{5}	-7. 45529 11365 07936 50793 65079 4 x 10^{6}	-6. 61211 50730 15873 01587 30158 7 x 10^{6}
8	-2. 45434 80000 00000 00000 00000 000 x 10^{6}	-1. 39686 45440 95238 09523 80952 4 x 10^{8}	-1. 21726 02948 25396 82539 68254 0 x 10^{8}
9	-4. 04557 92000 00000 00000 00000 000 x 10^{7}	-2. 65014 09796 83950 61728 39506 2 x 10^{9}	-2. 31846 76383 35097 00176 36684 3 x 10^{9}
10	-6. 76111 89000 00000 00000 00000 000 x 10^{8}	-5. 10616 90774 20007 05467 37213 4 x 10^{10}	-4. 66622 71320 45954 14462 08112 9 x 10^{10}
11	-1. 23090 34464 00000 00000 00000 000 x 10^{10}	-1. 04247 12453 03395 32467 53246 8 x 10^{12}	-9. 84809 97179 51261 69632 83629 9 x 10^{11}
12	-2. 38412 99211 60000 00000 00000 000 x 10^{11}	-2. 23016 29650 85629 37865 42675 4 x 10^{13}	-2. 14980 07877 36538 29768 58532 4 x 10^{13}
13	-4. 78926 88827 36000 00000 00000 000 x 10^{12}	-4. 91944 72964 29282 58912 11669 0 x 10^{14}	-4. 83496 01163 42960 68018 23690 7 x 10^{14}
14	-1. 00299 60764 62920 00000 00000 000 x 10^{14}	-1. 12225 28675 25768 45165 53217 5 x 10^{16}	-1. 12401 35072 47601 94486 12528 0 x 10^{16}
15	-2. 19391 40584 10784 00000 00000 000 x 10^{15}	-2. 65295 91858 70059 08542 19598 3 x 10^{17}	-2. 70125 37563 66712 47262 57043 4 x 10^{17}
16	-4. 98913 38393 59109 60000 00000 000 x 10^{16}	-6. 48199 61850 23826 22729 67446 6 x 10^{18}	-6. 69779 85890 44998 34046 32374 8 x 10^{18}
17	-1. 17721 33789 78895 71200 00000 000 x 10^{18}	-1. 63494 60327 61396 18599 43983 0 x 10^{20}	-1. 71247 09879 02293 66130 38586 9 x 10^{20}
18	-2. 88058 43388 66001 82580 00000 000 x 10^{19}	-4. 25659 28284 19743 45424 73387 8 x 10^{21}	-4. 51439 22010 11258 82664 38086 1 x 10^{21}
19	-7. 30209 82248 39883 55520 00000 000 x 10^{20}	-1. 14334 33867 13204 03393 45887 2 x 10^{23}	-1. 22655 00201 58564 38832 39288 5 x 10^{23}
20	-1. 91564 48562 67545 21945 00000 000 x 10^{22}	-3. 16673 73813 03954 79804 08780 5 x 10^{24}	-3. 43325 19223 39610 05699 60825 4 x 10^{24}
21	-5. 19690 13809 24973 96791 21600 000 x 10^{23}	-9. 04044 65735 66963 94912 61340 3 x 10^{25}	-9. 89740 68575 41075 34003 79363 9 x 10^{25}
22	-1. 45686 05280 77824 53021 96252 000 x 10^{25}	-2. 65909 74088 83205 00554 27661 4 x 10^{27}	-2. 93755 78773 17364 95086 14964 8 x 10^{27}
23	-4. 21719 12580 22755 91176 19011 200 x 10^{26}	-8. 05487 65908 80379 25062 66439 5 x 10^{28}	-8. 97310 57626 32034 42631 39732 5 x 10^{28}
24	-1. 25967 94654 24442 36755 85922 504 x 10^{28}	-2. 51173 13301 48609 92987 62592 6 x 10^{30}	-2. 81984 43774 15905 44331 56212 8 x 10^{30}
25	-3. 88002 45958 54034 72757 66618 730 x 10^{29}	-8. 05898 08749 29748 77315 30964 6 x 10^{31}	-9. 11294 89928 60760 81697 89730 6 x 10^{31}
26	-1. 23156 18914 48207 79510 27323 520 x 10^{31}	-2. 65934 77299 91991 69947 04818 7 x 10^{33}	-3. 02733 18655 21228 75404 05841 9 x 10^{33}
27	-4. 02566 98806 20394 69138 44635 383 x 10^{32}	-9. 02084 17726 16145 42317 13540 3 x 10^{34}	-1. 03332 27815 45672 51025 31966 2 x 10^{35}
28	-1. 35424 24210 16489 21939 79592 644 x 10^{34}	-3. 14397 93313 12732 90917 29422 5 x 10^{36}	-3. 62232 76612 73675 84487 97258 2 x 10^{36}
29	-4. 68544 75442 38667 24995 06874 748 x 10^{35}	-1. 12526 07148 86044 84077 11133 1 x 10^{38}	-1. 30350 01473 24107 21489 06879 0 x 10^{38}
30	-1. 66619 91081 12221 44530 75990 316 x 10^{37}	-4. 13376 48554 81829 50663 67925 6 x 10^{39}	-4. 81280 97930 09928 29278 75091 9 x 10^{39}
31	-6. 08631 04372 84698 90199 00511 196 x 10^{38}	-1. 55788 53861 85628 91404 25986 4 x 10^{41}	-1. 82239 14592 68996 77682 45153 6 x 10^{41}
32	-2. 28228 12507 85834 12798 16822 652 x 10^{40}	-6. 02006 93400 94138 15860 47590 2 x 10^{42}	-7. 07344 66737 29949 37561 84717 2 x 10^{42}
33	-8. 78042 25977 17389 15037 56947 826 x 10^{41}	-2. 38410 42750 50020 18495 10149 6 x 10^{44}	-2. 81293 24755 22493 31360 81692 0 x 10^{44}
34	-3. 46372 59781 60770 70431 46364 763 x 10^{43}	-9. 67145 13086 63695 32105 62437 6 x 10^{45}	-1. 14556 85717 78145 62829 08794 2 x 10^{46}
35	-1. 40026 99808 77340 28790 33201 661 x 10^{45}	-4. 01688 83158 69910 15916 67148 4 x 10^{47}	-4. 77545 13746 07933 01640 60098 4 x 10^{47}
36	-5. 79810 75784 61483 13779 28371 024 x 10^{46}	-1. 70731 38981 54727 92312 48876 2 x 10^{49}	-2. 03676 63980 95327 10302 79579 2 x 10^{49}
37	-2. 45776 83467 34762 55880 08187 252 x 10^{48}	-7. 42269 27067 44164 25656 63287 9 x 10^{50}	-8. 88398 42234 76867 67453 97625 6 x 10^{50}
38	-1. 06600 08819 26512 34909 70387 860 x 10^{50}	-3. 29942 67297 25793 16904 29985 3 x 10^{52}	-3. 96118 52062 63918 08076 63542 6 x 10^{52}
39	-4. 72852 35175 23039 41684 75576 411 x 10^{51}	-1. 49883 69874 28103 85887 03408 0 x 10^{54}	-1. 80471 79835 05179 76991 45339 9 x 10^{54}
40	-2. 14408 42507 99885 67706 80474 753 x 10^{53}	-6. 95544 43277 62059 42755 27395 3 x 10^{55}	-8. 39810 83786 08792 46629 11403 1 x 10^{55}
41	-9. 93369 12013 03364 97060 47121 705 x 10^{54}	-3. 29587 86844 69093 03980 22832 9 x 10^{57}	-3. 98995 29490 85868 17879 20812 8 x 10^{57}
42	-4. 70049 09765 31913 16033 29034 337 x 10^{56}	-1. 59411 73680 19089 84037 10866 1 x 10^{59}	-1. 93463 75203 34546 40507 16008 5 x 10^{59}
43	-2. 27068 85253 36619 89256 94923 984 x 10^{58}	-7. 86691 49377 51629 50970 48554 9 x 10^{60}	-9. 57003 21977 08557 92413 42140 9 x 10^{60}
44	-1. 11938 16860 65051 88188 31837 106 x 10^{60}	-3. 95969 18532 28589 44223 55991 9 x 10^{62}	-4. 82781 43119 36926 66208 37658 9 x 10^{62}
45	-5. 62905 98312 32797 88997 01881 543 x 10^{61}	-2. 03204 80899 73028 22339 94284 3 x 10^{64}	-2. 48288 92737 25694 54558 34330 0 x 10^{64}
46	-2. 88647 15078 74552 54081 55714 251 x 10^{63}	-1. 06284 55007 01580 81728 63182 1 x 10^{66}	-1. 30132 20428 94060 82772 51424 9 x 10^{66}
47	-1. 50874 14896 77968 88842 09398 943 x 10^{65}	-5. 66399 19589 73289 66761 01483 5 x 10^{67}	-6. 94845 83468 13190 87646 67923 7 x 10^{67}
48	-8. 03574 94933 05403 97340 21811 168 x 10^{66}	-3. 07431 88224 77668 01154 28549 8 x 10^{69}	-3. 77857 82063 30328 50661 93961 0 x 10^{69}
49	-4. 35968 37949 97962 43339 35268 334 x 10^{68}	-1. 69906 86683 08437 42409 10465 5 x 10^{71}	-2. 09203 52686 24217 27613 67235 4 x 10^{71}
50	-2. 40856 65421 69654 47050 34554 238 x 10^{70}	-9. 55817 58313 17034 50810 29931 8 x 10^{72}	-1. 17890 47292 28163 21278 91491 0 x 10^{73}
51	-1. 35456 58158 53828 79035 71962 601 x 10^{72}	-5. 47156 58928 71467 87770 00035 0 x 10^{74}	-6. 75974 05784 98781 49704 68065 1 x 10^{74}

obtained by summation of the asymptotic series.

As mentioned in the Introduction, proved in Ref. 6, and discussed in Sec. III I, the Borel sum of the RSPT series is the eigenvalue of the η equation [(11) or (16)] considered on a semi-infinite interval—that is, the ξ equation for the proton-antiproton-electron analog of $H_2{}^+$, analytically continued to negative $r'=e^{\pm\pi i}r$. We illustrate this fact by numerically solving Eq. (11) and comparing the results with the Borel sum of the RSPT. Also, as mentioned in the Introduction and elaborated in Sec. III I, the imaginary second-exponential-order series cancels (in that order) the imaginary part of the Borel sum. This too is illustrated numerically.

To solve the η equation [Eq. (11)] numerically is straightforward. There are two cases: the physical problem, for which the boundary conditions are

TABLE XIV. Coefficients for the RSPT series, the $\Delta E^{(1)}$ series, and the $\Delta_i E^{(2)}$ series, as defined by Eqs. (166), (234), and (235) of the text, for the $(n_1,n_2,m)=(0,0,1)$ excited state of H_2^+.

Order N	Coefficient $E^{(N)}$	$C^{(1)(N)}$	$C^{(2)(N)}$
0	-1.25000 00000 00000 00000 00000 000 × 10^{-1}	1.00000 00000 00000 00000 00000 000 × 10^{0}	1.00000 00000 00000 00000 00000 000 × 10^{0}
1	-1.00000 00000 00000 00000 00000 000 × 10^{0}	6.00000 00000 00000 00000 00000 000 × 10^{0}	1.20000 00000 00000 00000 00000 000 × 10^{1}
2	0.00000 00000 00000 00000 00000 000 × 10^{0}	-4.00000 00000 00000 00000 00000 000 × 10^{1}	-2.00000 00000 00000 00000 00000 000 × 10^{1}
3	6.00000 00000 00000 00000 00000 000 × 10^{0}	-3.13333 33333 33333 33333 33333 333 × 10^{2}	-9.30666 66666 66666 66666 66666 667 × 10^{2}
4	-7.80000 00000 00000 00000 00000 000 × 10^{1}	-6.36000 00000 00000 00000 00000 000 × 10^{2}	-3.88800 00000 00000 00000 00000 000 × 10^{3}
5	0.00000 00000 00000 00000 00000 000 × 10^{0}	-9.74346 66666 66666 66666 66666 667 × 10^{3}	4.25173 33333 33333 33333 33333 333 × 10^{3}
6	2.40000 00000 00000 00000 00000 000 × 10^{3}	-6.63105 77777 77777 77777 77777 778 × 10^{4}	-8.92423 11111 11111 11111 11111 111 × 10^{4}
7	-3.38880 00000 00000 00000 00000 000 × 10^{4}	-8.72937 90476 19047 61904 76190 476 × 10^{5}	-2.38107 58095 23809 52380 95238 095 × 10^{6}
8	-2.01552 00000 00000 00000 00000 000 × 10^{5}	-2.06407 56317 46031 74603 17460 317 × 10^{7}	-2.39404 25092 06349 20634 92063 492 × 10^{7}
9	1.83590 40000 00000 00000 00000 000 × 10^{6}	-1.64124 98162 68077 60141 09347 443 × 10^{8}	-2.93346 08305 89065 25573 19223 986 × 10^{8}
10	-2.84832 00000 00000 00000 00000 000 × 10^{7}	-2.09346 28756 24973 54497 35449 735 × 10^{9}	-4.63594 52763 15767 19576 71957 672 × 10^{9}
11	-5.03357 18400 00000 00000 00000 000 × 10^{8}	-5.70273 72832 45704 02437 06910 374 × 10^{10}	-7.85280 39569 21771 36443 80311 047 × 10^{10}
12	-3.22391 80800 00000 00000 00000 000 × 10^{8}	-7.52912 16606 84289 66917 85580 674 × 10^{11}	-1.25763 36191 02109 51846 50740 206 × 10^{12}
13	-6.05107 89120 00000 00000 00000 000 × 10^{10}	-1.10073 27081 05853 68409 36840 937 × 10^{13}	-2.07249 94023 45520 68612 86861 287 × 10^{13}
14	-1.55779 98520 32000 00000 00000 000 × 10^{12}	-2.56776 25455 98525 52148 33373 564 × 10^{14}	-3.96915 29593 73711 61752 43921 276 × 10^{14}
15	-1.55274 77514 24000 00000 00000 000 × 10^{13}	-4.67624 56349 41309 76112 04660 517 × 10^{15}	-7.63729 81098 86979 04298 51802 127 × 10^{15}
16	-3.55602 36364 87680 00000 00000 000 × 10^{14}	-8.69833 64731 46741 38952 49319 757 × 10^{16}	-1.48433 14650 21301 54467 04211 250 × 10^{17}
17	-8.45853 72059 68896 00000 00000 000 × 10^{15}	-1.94649 25960 50903 22910 74877 754 × 10^{18}	-3.14046 57783 86843 13845 77898 246 × 10^{18}
18	-1.55030 34534 60357 12000 00000 000 × 10^{17}	-4.23441 34580 44079 75888 46140 692 × 10^{19}	-6.88146 50168 65476 54439 58189 105 × 10^{19}
19	-3.47435 07633 56000 25600 00000 000 × 10^{18}	-9.47952 69136 31857 74985 45926 974 × 10^{20}	-1.55217 89615 30295 12284 42711 434 × 10^{21}
20	-8.26403 64221 95610 41920 00000 000 × 10^{19}	-2.27912 53793 21052 23534 50175 530 × 10^{22}	-3.68030 04405 46240 72734 18513 140 × 10^{22}
21	-1.93593 62616 33120 65740 80000 000 × 10^{21}	-5.62936 66395 36119 66727 47596 637 × 10^{23}	-9.06656 89837 58496 80487 69325 947 × 10^{23}
22	-4.83196 36650 94828 52352 00000 000 × 10^{22}	-1.44079 90980 28800 94926 31215 775 × 10^{25}	-2.31486 05013 69089 36122 67602 133 × 10^{25}
23	-1.25672 41823 94826 59550 00320 000 × 10^{24}	-3.84388 95512 42687 36148 29820 525 × 10^{26}	-6.14236 84542 90483 96293 16621 596 × 10^{26}
24	-3.37013 29576 46065 01404 26240 000 × 10^{25}	-1.06135 67327 59470 75379 34351 339 × 10^{28}	-1.68936 34595 43544 26784 87746 187 × 10^{28}
25	-9.39290 75638 92952 64919 65030 400 × 10^{26}	-3.03376 12021 30512 42240 06684 588 × 10^{29}	-4.81024 54768 03946 65503 88209 722 × 10^{29}
26	-2.71132 00561 65065 36836 23198 720 × 10^{28}	-8.97386 87029 24775 14417 97191 318 × 10^{30}	-1.41714 07609 16723 79689 97157 605 × 10^{31}
27	-8.09128 32612 42646 01222 90729 779 × 10^{29}	-2.74271 70573 43868 58021 36429 000 × 10^{32}	-4.31482 59411 72027 81563 48012 436 × 10^{32}
28	-2.49548 99420 83753 11255 23605 488 × 10^{31}	-8.65417 13474 22334 60100 18384 543 × 10^{33}	-1.35645 10024 47194 41857 90235 353 × 10^{34}
29	-7.94489 17212 85325 72940 45133 642 × 10^{32}	-2.81665 70663 08002 65701 39940 827 × 10^{35}	-4.39899 31536 84522 79913 57202 101 × 10^{35}
30	-2.60850 98915 74160 48759 40746 084 × 10^{34}	-9.44739 79326 16179 43050 82872 490 × 10^{36}	-1.47037 16906 69530 38102 56997 560 × 10^{37}
31	-8.82462 45508 00721 88099 02514 514 × 10^{35}	-3.26287 92722 86534 06252 05338 037 × 10^{38}	-5.06130 97420 74784 39918 58599 659 × 10^{38}
32	-3.07346 14862 62045 86105 09599 824 × 10^{37}	-1.15945 86093 45338 37345 86528 258 × 10^{40}	-1.79272 88486 36957 26310 14564 378 × 10^{40}
33	-1.10112 73649 30558 82575 59892 250 × 10^{39}	-4.23588 81092 84463 58024 43893 831 × 10^{41}	-6.52906 45911 03117 41294 04729 508 × 10^{41}
34	-4.05503 45195 29661 16680 23721 088 × 10^{40}	-1.58984 29830 77319 32496 31244 358 × 10^{43}	-2.44318 29183 87407 82755 20664 104 × 10^{43}
35	-1.53385 27913 91403 90547 20192 044 × 10^{42}	-6.12610 64551 10198 67769 01162 691 × 10^{44}	-9.38702 74388 65808 27712 41738 516 × 10^{44}
36	-5.95532 36273 01744 53409 88975 043 × 10^{43}	-2.42186 08439 48805 73956 79783 253 × 10^{46}	-3.70066 17534 38737 75273 38728 610 × 10^{46}
37	-2.37178 07899 28912 95636 13997 205 × 10^{45}	-9.81691 53742 78235 87270 35546 216 × 10^{47}	-1.49601 18442 71354 98293 15059 027 × 10^{48}
38	-9.68321 71094 63935 57357 24092 937 × 10^{46}	-4.07756 90855 82929 08603 15521 049 × 10^{49}	-6.19772 73227 03502 30614 23742 777 × 10^{49}
39	-4.05025 00974 05692 38867 98013 331 × 10^{48}	-1.73451 81709 06197 01771 38845 635 × 10^{51}	-2.62978 82798 73247 56954 59236 777 × 10^{51}
40	-1.73465 86175 36075 37666 46651 630 × 10^{50}	-7.55212 90343 61711 80522 56109 454 × 10^{52}	-1.14224 71213 20255 94148 37941 051 × 10^{53}
41	-7.60291 70182 24680 08150 85650 852 × 10^{51}	-3.36391 53585 79469 67683 86916 436 × 10^{54}	-5.07599 00458 59755 30397 78225 672 × 10^{54}
42	-3.40843 47604 02489 55538 60620 653 × 10^{53}	-1.53210 18169 00582 50921 85434 809 × 10^{56}	-2.30665 71954 95785 04387 82845 898 × 10^{56}
43	-1.56214 88856 74643 09257 31923 393 × 10^{55}	-7.13161 76542 23869 05167 95196 474 × 10^{57}	-1.07136 23139 48168 46122 10361 335 × 10^{58}
44	-7.31603 73911 17733 54980 96019 876 × 10^{56}	-3.39114 13767 52748 22306 21643 045 × 10^{59}	-5.08368 67259 82297 59093 05435 433 × 10^{59}
45	-3.49959 20366 93598 91668 17769 328 × 10^{58}	-1.64652 69780 08236 65118 91084 320 × 10^{61}	-2.46329 58768 55334 29456 33945 448 × 10^{61}
46	-1.70905 86893 95210 74016 63064 942 × 10^{60}	-8.15966 39046 03939 03795 80043 150 × 10^{62}	-1.21832 67347 46780 24063 44817 110 × 10^{63}
47	-8.51750 20559 09728 74946 57078 558 × 10^{61}	-4.12552 04419 46326 19565 13532 794 × 10^{64}	-6.14811 05845 66131 44197 51279 325 × 10^{64}
48	-4.33020 10973 72823 98193 60749 684 × 10^{63}	-2.12724 58801 31380 60942 97115 307 × 10^{66}	-3.16430 59699 84058 53906 59799 837 × 10^{66}
49	-2.24479 16414 87821 85905 65104 858 × 10^{65}	-1.11821 41806 45854 03997 46226 448 × 10^{68}	-1.66038 53659 20864 96222 15559 216 × 10^{68}
50	-1.18618 97135 90882 24223 81705 143 × 10^{67}	-5.99021 82780 86620 26463 55509 093 × 10^{69}	-8.87920 00375 59267 12556 46813 721 × 10^{69}
51	-6.38684 60774 93345 40838 33238 854 × 10^{68}	-3.26902 63820 18303 29932 40091 959 × 10^{71}	-4.83748 94548 79326 00323 72842 538 × 10^{71}

$\Phi_2(\eta)\sim\eta^{m/2+1/2}$ at $\eta=0$, and $\Phi_2(\eta)\sim(2-\eta)^{m/2+1/2}$ at $\eta=2$; and the semi-infinite problem for which the boundary condition at $\eta=2$ is replaced by $\Phi_2(\eta)\sim e^{-r\eta/2}$ as $\eta\to\infty$. In both cases the wave function near the origin can be expanded in a convergent power series in η. For the physical case, the power series can be summed at the midpoint of the physical interval, $\eta=1$, and the eigenvalue β_2 determined to make either Φ_2 or $d\Phi_2/d\eta$ vanish for odd or even states, respectively. For the unphysical case, $e^{r\eta/2}\Phi_2$ for large η can be expanded in a divergent series in powers of η^{-1}. This series can be summed to sufficient accuracy for the ground state for $|\eta|$ near 4, and then integrated numerically by a fourth-order Runge-Kutta algorithm[25] to a value of η for which the

TABLE XV. Asymptotic analysis of the RSPT $E^{(N)}$. The dominant, same-sign subseries in the asymptotic formula (236) of the text is truncated with the inclusion of the smallest term, whose index has been indicated by $k_{\min}$. The relative asymptotic error refers to the difference between the exact coefficient $E^{(N)}$ and the asymptotic formula to the indicated number of terms, divided by the leading asymptotic term, which is $-e^{-2n}(N+4n_2+2m+1)!/(n_2!)^2[(n_2+m)!]^2$. For sufficiently large N, the relative asymptotic error, after accounting for the same-sign subseries, is alternating in sign. The effect of the alternating-sign subseries is seen through the inclusion of up to three terms.

		same-sign subseries			alternating-sign subseries: relative asymptotic error after inclusion of terms through order (in N^{-1})		
N	$E^{(N)}$(exact)	$k_{\min}$	smallest term	relative asymptotic error	0	1	2
			Ground state: $n_1=0$, $n_2=0$, $m=0$				
20	-7.20352 71847 96734 02400 00000 000 × 10^{18}	9	1.4 × 10^{-4}	-3.0 × 10^{-5}	-5.2 × 10^{-5}	-4.3 × 10^{-5}	-3.8 × 10^{-5}
21	-1.58663 37018 30904 41984 00000 000 × 10^{20}	10	8.1 × 10^{-5}	1.1 × 10^{-5}	2.7 × 10^{-5}	2.1 × 10^{-5}	1.8 × 10^{-5}
22	-3.65198 45724 20448 69676 80000 000 × 10^{21}	10	4.6 × 10^{-5}	-9.5 × 10^{-6}	-2.2 × 10^{-5}	-1.7 × 10^{-5}	-1.5 × 10^{-5}
23	-8.76818 18011 54661 46806 40000 000 × 10^{22}	11	2.5 × 10^{-5}	-2.9 × 10^{-7}	8.7 × 10^{-6}	5.0 × 10^{-6}	3.9 × 10^{-6}
24	-2.19237 89692 87299 63470 43120 000 × 10^{24}	11	1.4 × 10^{-5}	-1.9 × 10^{-6}	-8.7 × 10^{-6}	-5.9 × 10^{-6}	-5.1 × 10^{-6}
25	-5.69988 90347 32373 98500 94080 000 × 10^{25}	12	7.8 × 10^{-6}	-1.8 × 10^{-6}	3.5 × 10^{-6}	1.2 × 10^{-6}	7.7 × 10^{-7}
26	-1.53868 45406 24901 90391 24834 560 × 10^{27}	12	4.3 × 10^{-6}	3.6 × 10^{-7}	-3.7 × 10^{-6}	-2.0 × 10^{-6}	-1.7 × 10^{-6}
27	-4.30701 59428 07344 63159 84849 344 × 10^{28}	13	2.4 × 10^{-6}	-1.5 × 10^{-6}	1.7 × 10^{-6}	3.5 × 10^{-7}	1.4 × 10^{-7}
28	-1.24856 46387 44255 27154 90329 645 × 10^{30}	13	1.3 × 10^{-6}	8.2 × 10^{-7}	-1.7 × 10^{-6}	-6.7 × 10^{-7}	-5.3 × 10^{-7}
29	-3.74403 87313 41340 10875 15630 039 × 10^{31}	14	7.0 × 10^{-7}	-1.1 × 10^{-6}	9.5 × 10^{-7}	1.1 × 10^{-7}	1.4 × 10^{-8}
30	-1.16009 28518 92770 55962 92709 845 × 10^{33}	14	3.8 × 10^{-7}	7.6 × 10^{-7}	-8.9 × 10^{-7}	-2.2 × 10^{-7}	-1.6 × 10^{-7}
45	-7.70037 25595 40304 33979 57208 022 × 10^{56}	22	2.9 × 10^{-11}	-8.6 × 10^{-8}	4.4 × 10^{-8}	-1.5 × 10^{-9}	-4.9 × 10^{-10}
60	-7.05864 08371 50714 38838 94260 882 × 10^{82}	30	1.7 × 10^{-15}	1.6 × 10^{-8}	-6.2 × 10^{-9}	3.5 × 10^{-10}	3.2 × 10^{-11}
75	-2.61042 76701 03107 25304 91597 603 × 10^{110}	37	8.3 × 10^{-20}	-4.2 × 10^{-9}	1.4 × 10^{-9}	-8.6 × 10^{-11}	-3.2 × 10^{-12}
90	-1.86576 07764 04173 29829 65438 924 × 10^{139}	45	3.8 × 10^{-24}	1.4 × 10^{-9}	-4.1 × 10^{-10}	2.5 × 10^{-11}	3.8 × 10^{-13}
105	-1.57799 46924 10063 42268 12311 752 × 10^{169}	51	1.7 × 10^{-28}	-5.7 × 10^{-10}	1.4 × 10^{-10}	-8.7 × 10^{-12}	-3.4 × 10^{-14}
120	-1.11215 08837 06133 49504 42764 523 × 10^{200}	51	2.3 × 10^{-32}	2.6 × 10^{-10}	-5.8 × 10^{-11}	3.4 × 10^{-12}	-8.7 × 10^{-15}
135	-5.01981 18745 10824 25602 25491 753 × 10^{231}	51	1.2 × 10^{-35}	-1.3 × 10^{-10}	2.6 × 10^{-11}	-1.5 × 10^{-12}	9.6 × 10^{-15}
150	-1.18207 97343 39949 69605 83966 744 × 10^{264}	51	1.7 × 10^{-38}	6.8 × 10^{-11}	-1.3 × 10^{-11}	7.0 × 10^{-13}	-6.3 × 10^{-15}
			Excited state: $n_1=1$, $n_2=0$, $m=0$				
35	-1.47781 93269 22509 49398 00218 784 × 10^{39}	23	2.1 × 10^{-9}	-5.5 × 10^{-3}	-3.3 × 10^{-3}	-4.8 × 10^{-3}	-6.8 × 10^{-3}
36	-5.42131 69465 84306 30428 52084 376 × 10^{40}	23	8.0 × 10^{-10}	1.1 × 10^{-3}	-7.4 × 10^{-4}	5.4 × 10^{-4}	2.0 × 10^{-3}
37	-2.03461 96166 09154 99124 05276 702 × 10^{42}	23	3.2 × 10^{-10}	-9.2 × 10^{-6}	1.5 × 10^{-3}	4.3 × 10^{-4}	-7.4 × 10^{-4}
38	-7.84562 80622 84487 21909 84822 569 × 10^{43}	23	1.3 × 10^{-10}	-2.6 × 10^{-5}	-1.3 × 10^{-3}	-3.9 × 10^{-4}	5.3 × 10^{-4}
39	-3.10431 97519 61902 94805 38840 486 × 10^{45}	23	5.5 × 10^{-11}	-5.5 × 10^{-5}	1.1 × 10^{-3}	2.4 × 10^{-4}	-4.7 × 10^{-4}
40	-1.25968 87575 41054 10432 57093 241 × 10^{47}	23	2.4 × 10^{-11}	8.5 × 10^{-5}	-8.6 × 10^{-4}	-1.6 × 10^{-4}	4.0 × 10^{-4}
41	-5.23747 50130 94393 89530 20851 158 × 10^{48}	23	1.1 × 10^{-11}	-8.7 × 10^{-5}	7.2 × 10^{-4}	1.2 × 10^{-4}	-3.3 × 10^{-4}
42	-2.23079 43468 42744 90353 52610 975 × 10^{50}	23	5.1 × 10^{-12}	8.2 × 10^{-5}	-6.1 × 10^{-4}	-9.5 × 10^{-5}	2.6 × 10^{-4}
43	-9.72417 45894 88816 20660 32201 663 × 10^{51}	23	2.4 × 10^{-12}	-7.6 × 10^{-5}	5.2 × 10^{-4}	7.4 × 10^{-5}	-2.1 × 10^{-4}
44	-4.33750 12238 23479 90153 12750 852 × 10^{53}	23	1.2 × 10^{-12}	7.2 × 10^{-5}	-4.5 × 10^{-4}	-5.8 × 10^{-5}	1.7 × 10^{-4}
45	-1.97804 24293 56898 01864 26922 166 × 10^{55}	23	6.0 × 10^{-13}	-6.7 × 10^{-5}	3.9 × 10^{-4}	4.5 × 10^{-5}	-1.4 × 10^{-4}
60	-1.65302 36911 22050 21932 71446 744 × 10^{81}	23	1.3 × 10^{-16}	2.1 × 10^{-5}	-5.5 × 10^{-5}	7.5 × 10^{-7}	1.0 × 10^{-5}
75	-5.76286 57185 48714 72612 15623 042 × 10^{108}	38	2.0 × 10^{-20}	-7.0 × 10^{-6}	1.2 × 10^{-5}	-9.5 × 10^{-7}	-1.3 × 10^{-6}
90	-3.95393 93851 27749 03143 18218 325 × 10^{137}	45	7.6 × 10^{-25}	2.7 × 10^{-6}	-3.7 × 10^{-6}	4.0 × 10^{-7}	2.5 × 10^{-7}
105	-3.24525 84385 46167 21188 41955 517 × 10^{167}	51	3.0 × 10^{-29}	-1.2 × 10^{-6}	1.3 × 10^{-6}	-1.6 × 10^{-7}	-5.9 × 10^{-8}
120	-2.23532 44929 47468 07900 46507 163 × 10^{198}	51	4.0 × 10^{-33}	5.6 × 10^{-7}	-5.4 × 10^{-7}	7.2 × 10^{-8}	1.6 × 10^{-8}
135	-9.90814 88516 78231 94553 22580 787 × 10^{229}	51	2.1 × 10^{-36}	-2.9 × 10^{-7}	2.5 × 10^{-7}	-3.4 × 10^{-8}	-5.2 × 10^{-9}
150	-2.29920 86344 61569 20265 54610 723 × 10^{262}	51	3.0 × 10^{-39}	1.6 × 10^{-7}	-1.2 × 10^{-7}	1.7 × 10^{-8}	1.8 × 10^{-9}
			Excited state: $n_1=0$, $n_2=1$, $m=0$				
90	-2.14579 08730 97608 03804 76312 533 × 10^{145}	44	7.2 × 10^{-20}	-2.4 × 10^{-20}	-3.9 × 10^{-20}	-2.3 × 10^{-20}	-2.9 × 10^{-20}
91	-2.06235 64052 64978 98704 71054 615 × 10^{147}	45	3.9 × 10^{-20}	3.0 × 10^{-22}	1.3 × 10^{-20}	-4.4 × 10^{-22}	4.8 × 10^{-21}
92	-2.00275 88289 87262 10407 16448 251 × 10^{149}	45	2.1 × 10^{-20}	-4.9 × 10^{-21}	-1.6 × 10^{-20}	-4.4 × 10^{-21}	-8.8 × 10^{-21}
93	-1.96488 19052 26077 10849 82754 451 × 10^{151}	46	1.1 × 10^{-20}	-1.7 × 10^{-21}	7.9 × 10^{-21}	-2.1 × 10^{-21}	1.6 × 10^{-21}
94	-1.94734 22525 53073 90685 34596 759 × 10^{153}	46	6.0 × 10^{-21}	1.4 × 10^{-22}	-8.2 × 10^{-21}	4.1 × 10^{-22}	-2.8 × 10^{-21}
95	-1.94940 56487 88341 35709 98583 644 × 10^{155}	47	3.2 × 10^{-21}	-1.9 × 10^{-21}	5.3 × 10^{-21}	-2.0 × 10^{-21}	6.5 × 10^{-22}
96	-1.97093 89906 90687 68548 88768 219 × 10^{157}	47	1.7 × 10^{-21}	1.2 × 10^{-21}	-4.9 × 10^{-21}	1.3 × 10^{-21}	-9.7 × 10^{-22}
97	-2.01239 36508 51118 68518 27733 602 × 10^{159}	48	9.1 × 10^{-22}	-1.6 × 10^{-21}	3.7 × 10^{-21}	-1.6 × 10^{-21}	3.3 × 10^{-22}
98	-2.07481 83306 90000 98785 56764 834 × 10^{161}	48	4.8 × 10^{-22}	1.3 × 10^{-21}	-3.3 × 10^{-21}	1.3 × 10^{-21}	-4.0 × 10^{-22}
99	-2.15990 16249 32295 06419 32336 636 × 10^{163}	49	2.6 × 10^{-22}	-1.2 × 10^{-21}	2.7 × 10^{-21}	-1.2 × 10^{-21}	2.0 × 10^{-22}
100	-2.27004 65857 57870 57892 29967 158 × 10^{165}	49	1.4 × 10^{-22}	1.1 × 10^{-21}	-2.4 × 10^{-21}	1.0 × 10^{-21}	-2.1 × 10^{-22}

TABLE XV. (*Continued*).

N	$E^{(N)}$(exact)	k_{min}	same-sign subseries: smallest term	same-sign subseries: relative asymptotic error	alternating-sign subseries: relative asymptotic error after inclusion of terms through order (in N^{-1}) 0	1	2
105	$-3.34887\,31765\,21245\,83788\,50242\,260 \times 10^{175}$	51	5.9×10^{-24}	-5.9×10^{-22}	1.1×10^{-21}	-5.1×10^{-22}	6.8×10^{-23}
110	$-6.19247\,66051\,35553\,60449\,62734\,926 \times 10^{185}$	51	2.9×10^{-25}	3.1×10^{-22}	-5.7×10^{-22}	2.5×10^{-22}	-3.7×10^{-23}
115	$-1.42134\,73900\,14061\,05461\,23906\,579 \times 10^{196}$	51	1.7×10^{-26}	-1.7×10^{-22}	3.0×10^{-22}	-1.2×10^{-22}	1.8×10^{-23}
120	$-4.01350\,46348\,84955\,00256\,59932\,505 \times 10^{206}$	51	1.2×10^{-27}	9.8×10^{-23}	-1.6×10^{-22}	6.4×10^{-23}	-9.5×10^{-24}
125	$-1.38280\,24776\,68477\,37271\,74455\,133 \times 10^{217}$	51	9.4×10^{-29}	-5.7×10^{-23}	8.7×10^{-23}	-3.4×10^{-23}	5.0×10^{-24}
130	$-5.76908\,79997\,60099\,90273\,22398\,986 \times 10^{227}$	51	8.3×10^{-30}	3.4×10^{-23}	-4.9×10^{-23}	1.9×10^{-23}	-2.7×10^{-24}
135	$-2.89404\,47723\,41030\,70694\,09814\,842 \times 10^{238}$	51	8.3×10^{-31}	-2.0×10^{-23}	2.8×10^{-23}	-1.0×10^{-23}	1.5×10^{-24}
140	$-1.73425\,01258\,17999\,54002\,35382\,259 \times 10^{249}$	51	9.1×10^{-32}	1.2×10^{-23}	-1.6×10^{-23}	6.0×10^{-24}	-8.6×10^{-25}
145	$-1.23389\,62504\,95032\,24434\,05554\,295 \times 10^{260}$	51	1.1×10^{-32}	-7.7×10^{-24}	9.8×10^{-24}	-3.5×10^{-24}	5.0×10^{-25}
150	$-1.03641\,42160\,91805\,70362\,06542\,761 \times 10^{271}$	51	1.5×10^{-33}	4.9×10^{-24}	-6.0×10^{-24}	2.1×10^{-24}	-2.9×10^{-25}
	Excited state: $n_1=0$, $n_2=0$, $m=1$						
45	$-3.49959\,20366\,93598\,91668\,17769\,328 \times 10^{58}$	22	7.5×10^{-10}	-2.7×10^{-10}	-6.6×10^{-10}	-2.4×10^{-10}	-1.7×10^{-10}
46	$-1.70905\,86893\,95210\,74016\,63064\,942 \times 10^{60}$	23	4.1×10^{-10}	-5.7×10^{-12}	3.0×10^{-10}	-2.9×10^{-11}	-7.6×10^{-11}
47	$-8.51750\,20559\,09728\,74946\,57078\,558 \times 10^{61}$	23	2.2×10^{-10}	-6.1×10^{-11}	-3.1×10^{-10}	-4.4×10^{-11}	-1.3×10^{-11}
48	$-4.33020\,10973\,72823\,98193\,60749\,684 \times 10^{63}$	24	1.2×10^{-10}	-1.8×10^{-11}	1.8×10^{-10}	-3.1×10^{-11}	-5.1×10^{-11}
49	$-2.24479\,16414\,87821\,85905\,65104\,858 \times 10^{65}$	24	6.4×10^{-11}	-3.6×10^{-12}	-1.6×10^{-10}	5.4×10^{-12}	1.8×10^{-11}
50	$-1.18618\,97135\,90882\,24223\,81705\,143 \times 10^{67}$	25	3.4×10^{-11}	-1.7×10^{-11}	1.1×10^{-10}	-2.4×10^{-11}	-3.2×10^{-11}
51	$-6.38684\,60774\,93345\,40838\,33238\,854 \times 10^{68}$	25	1.8×10^{-11}	9.3×10^{-12}	-9.6×10^{-11}	1.4×10^{-11}	1.8×10^{-11}
52	$-3.50285\,91147\,92997\,96351\,76467\,618 \times 10^{70}$	26	9.9×10^{-12}	-1.4×10^{-11}	7.2×10^{-11}	-1.7×10^{-11}	-1.9×10^{-11}
53	$-1.95622\,12316\,73804\,17530\,76068\,320 \times 10^{72}$	26	5.3×10^{-12}	1.0×10^{-11}	-6.1×10^{-11}	1.2×10^{-11}	1.3×10^{-11}
54	$-1.11207\,12695\,26913\,49760\,71599\,369 \times 10^{74}$	27	2.8×10^{-12}	-1.1×10^{-11}	4.8×10^{-11}	-1.2×10^{-11}	-1.2×10^{-11}
55	$-6.43326\,98100\,20438\,74103\,15384\,765 \times 10^{75}$	27	1.5×10^{-12}	8.6×10^{-12}	-4.0×10^{-11}	9.3×10^{-12}	8.5×10^{-12}
60	$-5.36148\,52495\,03114\,46697\,41902\,328 \times 10^{84}$	30	6.4×10^{-14}	-4.4×10^{-12}	1.5×10^{-11}	-4.0×10^{-12}	-2.7×10^{-12}
75	$-2.97729\,96882\,91636\,90670\,94542\,361 \times 10^{112}$	37	4.4×10^{-18}	6.1×10^{-13}	-1.4×10^{-12}	3.7×10^{-13}	1.2×10^{-13}
90	$-2.98060\,26338\,04127\,24387\,81243\,041 \times 10^{141}$	45	2.6×10^{-22}	-1.1×10^{-13}	2.0×10^{-13}	-5.2×10^{-14}	-8.1×10^{-15}
105	$-3.36203\,13361\,38534\,15647\,21639\,506 \times 10^{171}$	51	1.5×10^{-26}	2.7×10^{-14}	-3.8×10^{-14}	9.5×10^{-15}	7.4×10^{-16}
120	$-3.04696\,22545\,61093\,87351\,71675\,528 \times 10^{202}$	51	2.4×10^{-30}	-7.7×10^{-15}	9.2×10^{-15}	-2.2×10^{-15}	-7.0×10^{-17}
135	$-1.71925\,10469\,39378\,61467\,12246\,696 \times 10^{234}$	51	1.5×10^{-33}	2.5×10^{-15}	-2.6×10^{-15}	5.9×10^{-16}	2.3×10^{-18}
150	$-4.94850\,17433\,83943\,65938\,49553\,170 \times 10^{266}$	51	2.3×10^{-36}	-9.1×10^{-16}	8.5×10^{-16}	-1.8×10^{-16}	2.6×10^{-18}

series at the origin converges. The value of β_2 is determined by matching logarithmic derivatives. The integration path is kept away from $\eta=2$, at which the potential is singular, by keeping η in the lower half-plane. As a consequence, $\beta_2(r)$ for $r>0$ is continuous with $\mathrm{Im}\, r>0$. The numerical values of β_2 so obtained are listed in Table XVII.

To calculate the Borel sum is also straightforward.[26] For unimportant reasons of convenience, the values reported here were not calculated directly by the Borel method, but instead by the sequential Padé approximant method of Reinhardt,[27] which for the related problem of the LoSurdo-Stark effect in hydrogen[26,27] is known from numerical studies to give the same results as the Borel method. (The idea of this method is to generate the power-series expansion at some point away from the origin via Padé approximants of the series at the origin. At a point near the real axis in the right half-plane, β_2 is an analytic function of r, and the power series at that point converges on the nearby real axis. The procedure is most easily implemented in a continued-fraction representation of the RSPT series in which the even and odd approximants are the $[N/N]$ and $[N/N+1]$ Padé approximants,[26,28] We were able to calculate up to 70 continued-fraction coefficients for the function and its first 70 derivatives— using the RSPT coefficients through order 140—before completely losing numerical significance.) The numerical results are illustrated in Table XVII for the ground state at three internuclear distances. The values obtained by summing the RSPT series agree within the accuracy of the calculations with the values obtained by solving the differential equation numerically on the semi-infinite interval.

Summation of the imaginary second-exponential-order series for $\Delta_i\beta_2^{\{2\}}$ [Eq. (228)] and the real first-exponential-order series [Eq. (227)] is also reported in Table XVII. The sequential Padé-Padé method again was used, since these series are even more divergent than the RSPT series. Since only 51 power-series coefficients are available for these two series, Table I, the accuracy of the approximants for the higher derivatives is not as great as for the RSPT series. For $r=12$ and 10, the imaginary series cancels quite well the imaginary part of the Borel sum. For $r=6$, the cancellation is not so marked: clearly, higher-exponential-order series are not so small in the $r=6$ case and are needed to cancel the imaginary part of the Borel sum.

It should be noted that for each of the exponentially

TABLE XVI. Neville table for $-E^{(N)}/[e^{-2}(N+1)!]-1$ with up to three alternating-sign correction terms, for the ground state.

N	kth Neville iterate for k = 0	1	2	3	4
	with no alternating-sign correction term				
145	0.01282 68094 126	0.0009 887	−0.0000 199	−0.0003 504	−0.0253 500
146	0.01274 56323 515	0.0009 750	−0.0000 124	0.0003 444	0.0250 107
147	0.01266 54677 424	0.0009 614	−0.0000 190	−0.0003 365	−0.0246 785
148	0.01258 62975 623	0.0009 483	−0.0000 119	0.0003 308	0.0243 527
149	0.01250 81030 018	0.0009 353	−0.0000 182	−0.0003 233	−0.0240 335
150	0.01243 08668 759	0.0009 227	−0.0000 115	0.0003 179	0.0237 204
	with first alternating-sign correction term				
145	0.01282 68095 127	0.0009 887	−0.0000 156	0.0000 697	0.0050 078
146	0.01274 56322 555	0.0009 749	−0.0000 166	−0.0000 669	−0.0049 134
147	0.01266 54678 345	0.0009 615	−0.0000 149	0.0000 662	0.0048 212
148	0.01258 62974 739	0.0009 483	−0.0000 159	−0.0000 635	−0.0047 316
149	0.01250 81030 867	0.0009 353	−0.0000 143	0.0000 629	0.0046 440
150	0.01243 08667 944	0.0009 227	−0.0000 153	−0.0000 604	−0.0045 589
	with two alternating-sign correction terms				
145	0.01282 68094 954	0.0009 887	−0.0000 163	−0.0000 032	−0.0002 738
146	0.01274 56322 719	0.0009 749	−0.0000 159	0.0000 042	0.0002 678
147	0.01266 54678 188	0.0009 615	−0.0000 156	−0.0000 031	−0.0002 621
148	0.01258 62974 889	0.0009 483	−0.0000 152	0.0000 039	0.0002 564
149	0.01250 81030 724	0.0009 353	−0.0000 150	−0.0000 029	−0.0002 510
150	0.01243 08668 081	0.0009 227	−0.0000 146	0.0000 037	0.0002 456
	with three alternating-sign correction terms				
145	0.01282 68094 963	0.0009 887	−0.0000 163	0.0000 006	0.0000 021
146	0.01274 56322 711	0.0009 749	−0.0000 159	0.0000 005	−0.0000 022
147	0.01266 54678 196	0.0009 615	−0.0000 156	0.0000 005	0.0000 021
148	0.01258 62974 881	0.0009 483	−0.0000 153	0.0000 005	−0.0000 022
149	0.01250 81030 731	0.0009 353	−0.0000 150	0.0000 005	0.0000 021
150	0.01243 08668 074	0.0009 227	−0.0000 147	0.0000 004	−0.0000 022

small terms, the sum of each real power-series factor is itself also complex. However, here we have only listed the contribution that comes from the real part of the sum of each power-series factor, since the imaginary part would be expected to be canceled by higher-exponential-order series.

The sum of the first-exponential-order series can be either added or subtracted to the sum of the RSPT, leading to the symmetric or antisymmetric members of the double-well pair. Moreover, for quantitative accuracy, it is also necessary to include the real second-exponential-order series, for which we have given two terms in Eqs. (227) and (110), and which comes in only with one sign. The agreement of the sum of the asymptotic series with the numerical eigenvalues for the physical double-well pair is nicely illustrated for $r=12$ and 10, as well as the deteriorating convergence at $r=6$. At this shortest distance, the two-term truncation of the real second-exponential-order series is inadequate, and higher exponential-order contributions are also significant both for the accuracy of the real part and to cancel the imaginary part.

XII. SUMMARY

As set out in the Introduction, we have developed the quasisemiclassical method to solve the H_2^+ eigenvalue problem by asymptotic expansion. The bulk of the calculation has focused on the separation constants β_1 and β_2, which arise from separation in prolate spheroidal coordinates (Sec. II A). The transformation from separation constants to energy $E(R)$ is relatively elementary (Sec. V).

The development of asymptotic expansions for β_1 (Sec. IV) and β_2 (Sec. III) depends first on solving the separated Schrödinger equation near the boundary points, which are also singular points, in terms of Whittaker confluent hypergeometric functions. These solutions are extended away from the boundary points, by expanding the natural variable in a series in the reciprocal internuclear distance. The Schrödinger equation is thereby turned into a Riccati equation that is solved by expansion. A crucial role is played by the b index of the Whittaker function. If taken equal to the unperturbed separation constant, then RSPT is the result of solving the Riccati equation, but the wave function satisfies only the boundary condition at $\eta=0$. If

TABLE XVII. Comparison of values of β_2 obtained by summation of the asymptotic expansion and by numerical solution of the eigenvalue equation (11) with (physical) boundary conditions at $\eta=0$ and $\eta=2$, and with (nonphysical) boundary conditions at $\eta=0$ and $\eta=\infty$, for the ground state.

Computational Method	$\beta_2(r)$		
r=12			
Numerical solution, boundary conditions at 0 and $\infty - i\epsilon$	0.45620 55605 36	+ i 0.51348	x10^{-7}
Sequential Padé-Padé [35/35] for RSPT series	0.45620 55605 36	+ i 0.51347	x10^{-7}
Sequential Padé-Padé [25/26] for $\Delta\beta_2^{(1)}$	-0.00012 17975 46		
Sequential Padé-Padé [25/26] for $i\Delta_i\beta_2^{(2)}$		- i 0.51348	x10^{-7}
Two-term formula (110) for $\Delta_r\beta_2^{(2)}$	0.00000 01152 38		
RSPT + $\Delta\beta_2^{(1)}$ + $i\Delta_i\beta_2^{(2)}$ + $\Delta_r\beta_2^{(2)}$	0.45608 38782 28		
Sym. num. solution, boundary conditions at 0 and 2	0.45608 38789 89		
RSPT − $\Delta\beta_2^{(1)}$ + $i\Delta_i\beta_2^{(2)}$ + $\Delta_r\beta_2^{(2)}$	0.45632 74733 20		
Antisym. num. solution, boundary conditions at 0 and 2	0.45632 74743 50		
r=10			
Numerical solution, boundary conditions at 0 and $\infty - i\epsilon$	0.44675 97795 93	+ i 0.18165 34	x10^{-5}
Sequential Padé-Padé [35/35] for RSPT series	0.44675 97795 92	+ i 0.18165 34	x10^{-5}
Sequential Padé-Padé [25/26] for $\Delta\beta_2^{(1)}$	-0.00071 57275 4		
Sequential Padé-Padé [25/26] for $i\Delta_i\beta_2^{(2)}$		- i 0.18166	x10^{-5}
Two-term formula (110) for $\Delta_r\beta_2^{(2)}$	0.00000 37943		
RSPT + $\Delta\beta_2^{(1)}$ + $i\Delta_i\beta_2^{(2)}$ + $\Delta_r\beta_2^{(2)}$	0.44604 78463		
Sym. num. solution, boundary conditions at 0 and 2	0.44604 78627 33		
RSPT − $\Delta\beta_2^{(1)}$ + $i\Delta_i\beta_2^{(2)}$ + $\Delta_r\beta_2^{(2)}$	0.44747 93014		
Antisym. num. solution, boundary conditions at 0 and 2	0.44747 93660 55		
r=6			
Numerical solution, boundary conditions at 0 and $\infty - i\epsilon$	0.40438 98390 4	+ i 0.13374 2866	x10^{-2}
Sequential Padé-Padé [35/35] for RSPT series	0.40438 984	+ i 0.13374 3	x10^{-2}
Sequential Padé-Padé [25/26] for $\Delta\beta_2^{(1)}$	-0.01825 5		
Sequential Padé-Padé [25/26] for $i\Delta_i\beta_2^{(2)}$		- i 0.13508 0	x10^{-2}
Two-term formula (110) for $\Delta_r\beta_2^{(2)}$	0.00211 94		
RSPT + $\Delta\beta_2^{(1)}$ + $i\Delta_i\beta_2^{(2)}$ + $\Delta_r\beta_2^{(2)}$	0.38825 4	- i 0.00133 7	x10^{-2}
Sym. num. solution, boundary conditions at 0 and 2	0.38805 89412 28		
RSPT − $\Delta\beta_2^{(1)}$ + $i\Delta_i\beta_2^{(2)}$ + $\Delta_r\beta_2^{(2)}$	0.42476 5	- i 0.00133 7	x10^{-2}
Antisym. num. solution, boundary conditions at 0 and 2	0.42504 99757 82		

the boundary condition at $\eta=2$ is also to be satisfied, then the b index gains a sequence of exponentially small series, which in turn imply exponentially small contributions to the separation constant.

The explicit complexness of the expansions, starting in second exponential order, is a consequence of the explicit complexness of the asymptotic expansions for the Whittaker function. That a real function should have a complex asymptotic expansion is not as paradoxical as it might seem (Sec. III F): the asymptotic expansion for the Whittaker function is summable through the Borel summability of its associated power series. The real axis is a cut of the Borel sum. Thus the Borel sum of the RSPT series is complex and discontinuous on the real axis, but the explicit second-exponential-order series has the effect of canceling the implicit imaginary part and making the sum of the entire expansion (including all exponential orders) real and continuous.

The explicit imaginary series is directly related to the discontinuity on the positive real axis (Sec. III I) of the

Borel sum of RSPT for the separation constants, which in turn determines the asymptotics of the RSPT coefficients via a dispersion relation (Sec. VI). In the course of deriving the imaginary second-exponential-order expansion, the relation to the square of the first-exponential-order expansion is obtained, which is the exact version (Secs. III G and V C) of the approximate relation discovered by Brézin and Zinn-Justin.[12] There is also a second imaginary series (Sec. IV) associated with the discontinuity of β_1 on the negative r axis that leads both to alternating-sign and logarithmic contributions to the asymptotics of the RSPT coefficients (Sec. VI). These contributions had in fact implicitly been discovered in an earlier Bender-Wu analysis of the asymptotics of the RSPT for $H_2{}^+$.[13]

Extensive numerical illustration has been provided for both the values (Tables I—III, V—VIII, and XI—XIV) and the asymptotic behavior (Tables IV, X, XV, and XVI) of the coefficients of the various series. In particular, the relation between the imaginary series and the RSPT asymptotics is verified in practice (Tables IV, X, XV, and XVI). The higher the quantum numbers n_1 and n_2 the more slowly the RSPT approaches asymptotic behavior. The alternating-sign contributions to both $\beta_1^{(N)}$ and to $E^{(N)}$ have been explicitly demonstrated (Tables X, XV, and XVI).

The RSPT series for β_2 has been summed and shown (Table XVII) to agree numerically with the numerical solution of the differential equation for β_2 on a semi-infinite domain, the analytic continuation to negative r' or the closely related $\beta_1'(r')$ for the electron moving in the field of a proton and an antiproton. For instance, at $r=10$ the sum of the RSPT series for β_2 is $0.446\,759\,779\,592+i\,0.181\,653\,4\times10^{-5}$, while direct numerical integration of the differential equation gives $0.446\,759\,779\,593+i\,0.181\,653\,4\times10^{-5}$. For the physical β_2, the sum of all the β_2 subseries together agrees well with the numerically solved values for β_2 for large r (≥ 10), but still more terms and subseries are needed for smaller r ($r=6$ being the example given in Table XVII).

Such a richly complex asymptotic expansion for such a simple problem was not anticipated.

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