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Anharmonic oscillator discontinuity formulae up to second-exponentially-small order

Gabriel Álvarez¹, Christopher J Howls² and Harris J Silverstone³

¹ Departamento de Física Teórica II, Facultad de Ciencias Físicas, Universidad Complutense, 28040 Madrid, Spain

² Faculty of Mathematical Studies, University of Southampton Highfield, Southampton SO17 1BJ, UK

³ Department of Chemistry, The Johns Hopkins University, Baltimore, MD 21218, USA

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Abstract

The eigenvalues of the quartic anharmonic oscillator as functions of the anharmonicity constant satisfy a once-subtracted dispersion relation. In turn, this dispersion relation is driven by the purely imaginary discontinuity of the eigenvalues across the negative real axis. In this paper we calculate explicitly the asymptotic expansion of this discontinuity up to second-exponentially-small order.

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1. Introduction

There has been increasing interest of the mathematical physics community in the derivation and interpretation of asymptotic expansions that take into account the exponentially small terms sometimes neglected by the Poincaré definition of asymptotic power series [1]. In the companion paper [2] we study the derivation of the so-called hyperasymptotic expansions for the eigenvalues of the anharmonic oscillator. Such expansions differ from ordinary asymptotics by considering the global behaviour of the progenitor function. The result is a systematic algorithm to obtain a uniform sequence of exponentially accurate expansions valid over increasingly larger ranges of the asymptotic parameter.

To date, hyperasymptotics has been performed for the solutions of certain classes of differential equations [3–5], but not for individual eigenvalues. Furthermore, the study of anharmonic eigenvalues illustrates an extension of hyperasymptotics to functions which may not have an explicit integral representation, but instead satisfy a dispersion relation. As we discuss in detail in [2], there is no known integral representation for the eigenvalues of this anharmonic oscillator. However, if we first subtract the unperturbed (harmonic) eigenvalue

$E_n^{(0)} = n + 1/2$ from the anharmonic eigenvalue $E_n(g)$, the latter can be expressed as a ‘once-subtracted dispersion relation’ [6, 7] in the coupling constant g ,

$$E_n(g) = E_n^{(0)} + \frac{(-g)}{2\pi i} \int_0^\infty \frac{\Delta E_n(z)}{z(z+g)} dz \quad (1)$$

where

$$\Delta E_n(z) \equiv E_n(e^{-i\pi} z) - E_n(e^{+i\pi} z) \quad (2)$$

denotes the purely imaginary discontinuity of the eigenvalue $E_n(g)$ across the negative coupling-constant axis. Inserting the geometric sum

$$\frac{(-g)}{z(z+g)} = -\frac{g}{z^2} + \frac{g^2}{z^3} - \dots + (-1)^{N_0-1} \frac{g^{N_0-1}}{z^{N_0}} + (-1)^{N_0} \frac{g^{N_0}}{z^{N_0}(z+g)} \quad (3)$$

into the dispersion relation (1) gives rise to an exact expression for the Rayleigh–Schrödinger (RS) partial sum with remainder

$$E_n(g) = \sum_{j=0}^{N_0-1} E_n^{(j)} g^j + R_n(N_0, g) \quad (4)$$

$$R_n(N_0, g) = \frac{(-1)^{N_0} g^{N_0}}{2\pi i} \int_0^\infty \frac{z^{-N_0}}{z+g} \Delta E_n(z) dz. \quad (5)$$

By simply dropping the remainder $R_n(N_0, g)$ in equation (4) we would just recover the standard RS asymptotic power series, but by a suitable recursive procedure that takes into account the analytic properties of the discontinuity $\Delta E_n(z)$, we are led to the systematic sequence of hyperasymptotic expansions previously mentioned.

Two ingredients are required to generate a hyperasymptotic expansion: the first is the sequence of local expansions about the discontinuities in the dispersion relation of a particular problem; the second is the recursive insertion, manipulation and evaluation of these expansions into the dispersion relation. (The latter procedure is generic.)

The purpose of the present paper is therefore to discuss the analytic properties and to calculate explicitly the asymptotic expansion of the discontinuity $\Delta E_n(z)$ up to second-exponentially-small order for the particular problem of a quartically perturbed anharmonic oscillator. The companion paper [2] details the subsequent hyperasymptotic manipulation for eigenvalue problems, albeit exemplified by the quartic oscillator. To emphasize the distinction between these two ingredients, we have split the work accordingly.

The basic idea for this calculation is contained in [8], and is fully developed in section 2: to match two Borel-summable asymptotic expansions for the wavefunction (built around the origin and around the outer turning point, respectively) in the intermediate ‘under the barrier’ region. Matching on the first sheet of the coupling constant plane recovers the Borel-summable RS series, but matching on the second sheet gives a different, more complicated expansion, which consists of the RS series plus an infinite sequence of successively exponentially smaller subseries. Both kinds of expansions are required to calculate the discontinuity of the energy. (Incidentally, in section 2 we give the full matching condition—which was only implicit in [8]—although we solve it explicitly only up to second-exponentially-small order.) In section 3 we illustrate an indirect but very efficient method for the evaluation of the coefficients of the main series that appears in the matching condition. We do not have a proof of the corresponding equation (which was noted in a different context by Hoe *et al* [9]); we have checked it up to order 10. Section 4 contains formulae for the coefficients of the rest of the series as functions of the coefficients of the main series calculated in section 3, as well as

an analysis of the asymptotic behaviour of these coefficients. This asymptotic behaviour is necessary to estimate the optimum truncations of the hyperasymptotic series obtained in [2]. The paper ends with a brief summary.

2. Derivation of the discontinuity formulae

The quartic anharmonic oscillator is characterized by the Schrödinger equation

$$\left[-\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2}x^2 + gx^4 - E(g) \right] \psi(x) = 0 \tag{6}$$

with boundary conditions $\psi(\pm\infty) = 0$. The change of variables

$$\sigma = x^2 \tag{7}$$

$$\psi(x) = \sigma^{-1/4} \Phi(\sigma) \tag{8}$$

in the Schrödinger equation (6) yields

$$\left[-\sigma \frac{d^2}{d\sigma^2} - \frac{3}{16\sigma} + \frac{1}{4}\sigma + \frac{1}{2}g\sigma^2 - \frac{1}{2}E(g) \right] \Phi(\sigma) = 0 \tag{9}$$

where the transformed boundary conditions are $\Phi(0) = \Phi(+\infty) = 0$. Near the origin, where the term $\frac{1}{2}g\sigma^2$ becomes negligible, equation (9) reduces to Whittaker’s differential equation [10], while for large σ we may drop the $-3/(16\sigma)$ and $-E(g)/2$ terms, and equation (9) reduces to Airy’s differential equation [10]. Taking these Whittaker and Airy equations as unperturbed comparison equations, and using ideas of Langer [11] and Cherry [12], we build two corresponding asymptotic expansions that have to be matched in the intermediate region.

2.1. Asymptotic expansion anchored at the origin

As discussed in [8], to build the origin-anchored solution we scale the independent variable in equation (9) by

$$y = g^{1/2}\sigma \tag{10}$$

so that the unperturbed problem near the origin is the harmonic oscillator, the anharmonicity term is a first-order perturbation in $g^{1/2}$, and the Schwarzian derivative enters at second order. We write the Langer–Cherry form of the wavefunction as

$$\Phi(\sigma) = \left(\frac{d\phi_0}{dy} \right)^{-1/2} M_{\frac{w}{2} + \frac{1}{4}, -\frac{1}{4} + \frac{\delta}{2}}(g^{-1/2}\phi_0(y)) \tag{11}$$

where $M_{\kappa,\mu}(\sigma)$ is Whittaker’s confluent hypergeometric function [10] and where $\delta = 0$ for even solutions and $\delta = 1$ for odd solutions. (The harmonic oscillator wavefunctions are given by $M_{\frac{w}{2} + \frac{1}{4}, -\frac{1}{4}}(\sigma)$ for n even, and $M_{\frac{w}{2} + \frac{1}{4}, \frac{1}{4}}(\sigma)$ for n odd.) Note also the as yet unspecified parameter w in the first index of the Whittaker function. We will see that the matching condition is in fact an equation for this parameter [8, 13, 14].

Substituting equations (10) and (11) into equation (9) we find a differential equation for ϕ_0

$$\begin{aligned} \left(\frac{d\phi_0}{dy} \right)^2 \left[\frac{1}{4} - g \frac{3}{16} \frac{1}{\phi_0^2} - \frac{1}{2}g^{1/2} \left(w + \frac{1}{2} \right) \frac{1}{\phi_0} \right] &= \frac{1}{4} - \frac{1}{2}g^{1/2} \frac{E}{y} + \frac{1}{2}g^{1/2}y - g \frac{3}{16} \frac{1}{y^2} \\ &- g \left(\frac{d\phi_0}{dy} \right)^{1/2} \frac{d^2}{dy^2} \left(\frac{d\phi_0}{dy} \right)^{-1/2}. \end{aligned} \tag{12}$$

We solve this equation by asymptotic expansion of ϕ_0 :

$$\phi_0(y) \sim \sum_{N=0}^{\infty} g^{N/2} \phi_0^{(N/2)}(y) \quad (13)$$

and of the energy:

$$E(g) \sim \sum_{N=0}^{\infty} g^{N/2} E_w^{(N/2)}. \quad (14)$$

The condition that ϕ_0 be regular at the origin implies that the $E_w^{(N/2)}$ vanish for N odd, and fixes the values of the $E_w^{(N/2)}$ for N even, which turn out to be polynomials in the unspecified parameter w [8]. The integrations can be performed explicitly, and for later reference we give the first two terms of the expansion (13):

$$\phi_0^{(0)}(y) = y \quad (15)$$

$$\phi_0^{(1/2)}(y) = \frac{1}{2}y^2 \quad (16)$$

and the first four non-vanishing terms of the energy expansion (14)

$$E_w^{(0)} = w + \frac{1}{2} \quad (17)$$

$$E_w^{(1)} = \frac{3}{2}w^2 + \frac{3}{2}w + \frac{3}{4} \quad (18)$$

$$E_w^{(2)} = -\frac{17}{4}w^3 - \frac{51}{8}w^2 - \frac{59}{8}w - \frac{21}{8} \quad (19)$$

$$E_w^{(3)} = \frac{375}{16}w^4 + \frac{375}{8}w^3 + \frac{177}{2}w^2 + \frac{1041}{16}w + \frac{333}{16}. \quad (20)$$

2.2. Asymptotic expansion anchored at the outer turning point

Similarly, we build a Langer–Cherry asymptotic expansion anchored at the outer turning point, except that we scale now

$$\zeta = 2g\sigma \quad (21)$$

so that the anharmonic term is of zeroth order in g and the shorter-range terms become the perturbation [8]. We write the wavefunction in the form

$$\Phi(\sigma) = 2\pi^{1/2}(4g)^{-1/6} \left(\frac{d\phi_\infty}{d\zeta} \right)^{-1/2} \text{Ai} \left((4g)^{-2/3} \phi_\infty(\zeta) \right) \quad (22)$$

where $\text{Ai}(z)$ is Airy's function [10] and the ζ -independent prefactors simplify the form of the asymptotic expansions. The resulting differential equation for ϕ_∞ is

$$\left(\frac{d\phi_\infty}{d\zeta} \right)^2 \phi_\infty = 1 + \zeta - g \frac{4E}{\zeta} - g^2 \frac{3}{\zeta^2} - 16g^2 \left(\frac{d\phi_\infty}{d\zeta} \right)^{1/2} \frac{d^2}{d\zeta^2} \left(\frac{d\phi_\infty}{d\zeta} \right)^{-1/2} \quad (23)$$

which again we solve by expansion of the energy (equation (14)) and of ϕ_∞ as asymptotic power series in g

$$\phi_\infty(\zeta) \sim \sum_{N=0}^{\infty} g^N \phi_\infty^{(N)}(\zeta). \quad (24)$$

(Note the consistency of the procedure that follows from the vanishing of the $E_w^{(N/2)}$ for N odd.) For later reference we give explicitly the first two terms of equation (24)

$$\phi_\infty^{(0)}(\zeta) = 1 + \zeta \quad (25)$$

$$\phi_\infty^{(1)}(\zeta) = -(2w+1)(1+\zeta)^{-1/2} \ln \left[\frac{1 - (1+\zeta)^{1/2}}{1 + (1+\zeta)^{1/2}} \right]. \quad (26)$$

(The parameter w enters $\phi_\infty^{(1)}(\zeta)$ via the asymptotic expansion of the energy (14) that has been substituted into equation (23).)

2.3. Borel-summable asymptotic expansions

The Borel-summable asymptotic expansions for the confluent hypergeometric functions $M_{\kappa,\mu}(\sigma)$ have been discussed in [15], to which we refer especially for a detailed treatment of the domains of summability. By making use of the gamma function reflection and duplication formulae [10], the asymptotic expansion for the origin-anchored wavefunction (11) can be written as

$$\begin{aligned} \Phi(\sigma) \sim & \left(\frac{d\phi_0}{dy}\right)^{-1/2} e^{-g^{1/2}\phi_0/2} \Gamma\left(\frac{1}{2} + \delta\right) \Gamma\left(1 + \frac{1}{2}(w - \delta)\right) e^{\mp i\pi(w-\delta)/2} \\ & \times \left[\frac{2^{w+1/2}}{(2\pi)^{1/2}\Gamma(w+1)} (g^{-1/2}\phi_0)^{\frac{w}{2}+\frac{1}{4}} {}_2F_0\left(-\frac{w}{2}, \frac{1}{2} - \frac{w}{2}; ; -\frac{g^{1/2}}{\phi_0}\right) \right. \\ & \left. \pm \frac{i}{2\pi} (e^{\pm i\pi(w-\delta)} - 1) e^{g^{-1/2}\phi_0} (g^{-1/2}\phi_0)^{-\frac{w}{2}-\frac{1}{4}} {}_2F_0\left(\frac{1}{2} + \frac{w}{2}, 1 + \frac{w}{2}; ; \frac{g^{1/2}}{\phi_0}\right) \right] \end{aligned} \tag{27}$$

where the upper signs are valid for $0 < \arg(g^{-1/2}\phi_0) < \pi$ and the lower signs for $-\pi < \arg(g^{-1/2}\phi_0) < 0$. But using equations (10), (15) and (16) we see that

$$\arg(g^{-1/2}\phi_0) \sim \arg\left[\sigma + \frac{g}{2}\sigma^2\right] \tag{28}$$

and if everything else is real

$$\operatorname{sgn}[\operatorname{Im}(g^{-1/2}\phi_0)] = \operatorname{sgn}[\operatorname{Im}g]. \tag{29}$$

Therefore, the upper signs in equation (27) hold for $\operatorname{Im}g > 0$ and the lower signs for $\operatorname{Im}g < 0$.

The asymptotic expansion for the Airy-based wavefunction is slightly more complicated [8]. If

$$|\arg((4g)^{-2/3}\phi_\infty)| < \frac{2\pi}{3} \tag{30}$$

that is to say, if

$$|\arg g| < \pi \tag{31}$$

then

$$\Phi(\sigma) \sim \left(\frac{d\phi_\infty}{d\zeta}\right)^{-1/2} \phi_\infty^{-1/4} e^{-(6g)^{-1}\phi_\infty^{3/2}} {}_2F_0\left(\frac{1}{6}, \frac{5}{6}; ; -\frac{3g}{\phi_\infty^{3/2}}\right). \tag{32}$$

However, as soon as

$$\mp \arg g = \pi + \epsilon > \pi \tag{33}$$

which for convenience we will write in the form

$$g = z e^{\mp i\pi} \quad (\arg z = \mp \epsilon) \tag{34}$$

then

$$\begin{aligned} \Phi(\sigma) \sim & \left(\frac{d\phi_\infty}{d\zeta}\right)^{-1/2} \phi_\infty^{-1/4} \left[e^{(6z)^{-1}\phi_\infty^{3/2}} {}_2F_0\left(\frac{1}{6}, \frac{5}{6}; ; \frac{3z}{\phi_\infty^{3/2}}\right) \right. \\ & \left. \pm i e^{-(6z)^{-1}\phi_\infty^{3/2}} {}_2F_0\left(\frac{1}{6}, \frac{5}{6}; ; -\frac{3z}{\phi_\infty^{3/2}}\right) \right]. \end{aligned} \tag{35}$$

2.4. Matching

If $|\arg g| < \pi$, then the asymptotic expansion (32) has a single exponential subseries. To match the compound asymptotic expansion (27), the second subseries in the latter must vanish. Therefore we must have $e^{\pm i\pi(w-\delta)} = 1$ in equation (27) or

$$w = n \quad (n = 0, 1, \dots) \quad (36)$$

and the asymptotic expansion for the energy (14) takes the form

$$E_n(g) \sim \sum_{j=0}^{\infty} E_n^{(j)} g^j \equiv E_n^{\text{RS}}(g) \quad (|\arg g| < \pi) \quad (37)$$

which is precisely the Borel-summable power series for $E_n(g)$. In particular, we recover the well-known result that the RS coefficients $E_n^{(j)}$ are polynomials of degree $j+1$ in the harmonic oscillator quantum number. We stress, however, that these polynomials have been obtained from the *general* asymptotic expansion for the energy (14) by setting $w = n$.

But if $\arg g = -\pi - \epsilon < -\pi$ and therefore falls in the second quadrant of the next clockwise sheet, then both exponentials are present in the ϕ_∞ wavefunction, and the matching process implies an exponentially small contribution to w ,

$$w = n + \Delta w_-(n, z) \quad (g = e^{-i\pi} z \quad \arg z = -\epsilon < 0) \quad (38)$$

while if $\arg g = \pi + \epsilon > \pi$ and therefore falls in the third quadrant of the next anticlockwise sheet, then the matching process implies that

$$w = n + \Delta w_+(n, z) \quad (g = e^{i\pi} z \quad \arg z = \epsilon > 0). \quad (39)$$

That is, $|\arg g| = \pi$ is a Stokes line for the energy eigenvalue: the usual RS expansion changes to one formally derived from the general RS expansion by replacing n by $n + \Delta w_\mp$ depending on whether the negative axis is crossed in the clockwise or anticlockwise direction.

The matching condition is obtained by equating the ratios of the dominant to the subdominant terms in the two asymptotic expansions (27) and (35). This condition can be written in the form [13]

$$\begin{aligned} \Delta w_\mp(n, z) &= \mp \frac{i}{\pi} \ln [1 + \pi B(n + \Delta w_\mp, z) f(n + \Delta w_\mp, z)] \\ (g = e^{\mp i\pi} z \quad \arg z = \mp \epsilon \quad \epsilon > 0) \end{aligned} \quad (40)$$

where

$$B(w, z) = 2\pi C_w (3z)^{-w-\frac{1}{2}} e^{-\frac{1}{3z}} \quad (41)$$

$$C_w = \frac{12^{w+\frac{1}{2}}}{\pi \sqrt{2\pi} \Gamma(w+1)} \quad (42)$$

$$\begin{aligned} f(w, z) &= \left(\frac{\phi_0}{y}\right)^{w+\frac{1}{2}} \exp[g^{-1/2}(y - \phi_0)] \\ &\times \exp\left[-(3z)^{-1} \left(\phi_\infty^{3/2} - 1 + 3z\sigma - 3z \left(w + \frac{1}{2}\right) \ln\left(\frac{z\sigma}{2}\right)\right)\right] \\ &\times \frac{{}_2F_0\left(\frac{1}{6}, \frac{5}{6}; ; -\frac{3z}{\phi_\infty^{3/2}}\right) {}_2F_0\left(-\frac{w}{2}, \frac{1}{2} - \frac{w}{2}; ; -\frac{g^{1/2}}{\phi_0}\right)}{{}_2F_0\left(\frac{1}{6}, \frac{5}{6}; ; \frac{3z}{\phi_\infty^{3/2}}\right) {}_2F_0\left(\frac{1}{2} + \frac{w}{2}, 1 + \frac{w}{2}; ; \frac{g^{1/2}}{\phi_0}\right)}. \end{aligned} \quad (43)$$

A few comments are in order. First note that the even-odd parameter δ has disappeared in the omitted intermediate transformations, due to the fact that $n - \delta$ is always an even integer.

Second, note that the matching function $f(w, z)$ is independent of σ , and that we have used the explicit form of the two lowest orders of ϕ_0 and ϕ_∞ to pull out the exponentially small leading behaviour in the form of the prefactor $B(w, z)$. Using *Mathematica*, we have implemented the procedure outlined in this section and calculated $f(w, z)$ as a power series in z through order z^{10} , with coefficients as polynomials in w . It turns out that the coefficient of z^k is a polynomial in w of degree $2k$:

$$f(w, z) = 1 - z \left(\frac{59}{24} + \frac{17}{4}w + \frac{17}{4}w^2 \right) + z^2 \left(-\frac{9011}{1152} - \frac{1829}{96}w - \frac{95}{24}w^2 + \frac{39}{16}w^3 + \frac{289}{32}w^4 \right) + O(z^3). \tag{44}$$

After equation (40) has been solved for Δw_\mp , we can write formally the asymptotic expansion for the energy $E_n(g)$ as

$$E_n(g) \sim \exp(\Delta w_\mp \partial / \partial n) E_n^{\text{RS}}(g) \quad (\arg g = \mp \pi \mp \epsilon) \tag{45}$$

where Δw_\mp is held constant with respect to $\partial / \partial n$.

2.5. Iterative solution for $\Delta w_\mp(n, z)$

Equation (40) permits an iterative solution, which in this paper we carry out explicitly to second order. Note that $B(w, z)$ contains the exponentially small factor $\exp[-1/(3z)]$. To keep track of its powers, we introduce a variable of convenience λ , then rewrite equation (40) and expand Δw_\pm in powers of λ (which can be set equal to 1 at the end)

$$\Delta w_\mp(n, z) = \lambda \Delta w_\mp^{\{1\}} + \lambda^2 \Delta w_\mp^{\{2\}} + \dots \tag{46}$$

$$= \mp \frac{i}{\pi} \ln \{ 1 + \pi \exp(\Delta w_\mp \partial / \partial n) [\lambda B(n, z) f(n, z)] \} \tag{47}$$

$$= \mp \lambda i B f + \lambda^2 \left(\frac{\pm i \pi}{2} B^2 f^2 \mp i \Delta w_\mp^{\{1\}} \frac{\partial}{\partial n} B f \right) + O(\lambda^3). \tag{48}$$

From equations (46) and (48) we obtain $\Delta w_\mp^{\{1\}}$ and $\Delta w_\mp^{\{2\}}$:

$$\Delta w_\mp^{\{1\}} = \mp i B(n, z) f(n, z) \tag{49}$$

$$\Delta w_\mp^{\{2\}} = \pm i \frac{\pi}{2} B^2 f^2 - B f \frac{\partial}{\partial n} B f \tag{50}$$

$$= \pm i \frac{\pi}{2} B(n, z)^2 f(n, z)^2 + B(n, z)^2 \left\{ f(n, z)^2 \left[\ln \left(\frac{z}{4} \right) + \psi(n + 1) \right] - f(n, z) \frac{\partial f(n, z)}{\partial n} \right\}. \tag{51}$$

2.6. Solution for $\Delta E_n^{\{k\}}$ in terms of $\Delta w_\mp^{\{j\}}$

The asymptotic expansion for the energy discontinuity is obtained from equations (37) and (45), with equations (49) and (51) for $\Delta w_\mp^{\{1\}}$ and $\Delta w_\mp^{\{2\}}$. Since the negative g axis is a Stokes line, the expansions in the second and third quadrants are different. In the second quadrant $\arg z = -\epsilon < 0$, and $g = e^{-i\pi} z$ requires equation (45) with the upper sign, while $g = e^{+i\pi} z$ requires equation (37)

$$\Delta E_n(z) = E_n(e^{-i\pi} z) - E_n(e^{+i\pi} z) \tag{52}$$

$$\sim [\exp(\Delta w_-(n, z) \partial / \partial n) - 1] E_n^{\text{RS}}(-z) \tag{53}$$

$$= \Delta w_- \frac{\partial}{\partial n} E_n^{\text{RS}}(-z) + \frac{1}{2} (\Delta w_-)^2 \frac{\partial^2}{\partial n^2} E_n^{\text{RS}}(-z) + \dots \quad (54)$$

$$= \lambda \Delta w_-^{(1)} \frac{\partial}{\partial n} E_n^{\text{RS}}(-z) + \lambda^2 \left[\Delta w_-^{(2)} \frac{\partial}{\partial n} E_n^{\text{RS}}(-z) + \frac{1}{2} (\Delta w_-^{(1)})^2 \frac{\partial^2}{\partial n^2} E_n^{\text{RS}}(-z) \right] + O(\lambda^3). \quad (55)$$

In the third quadrant $\arg z = +\epsilon > 0$, and $g = e^{-i\pi} z$ requires equation (37), while $g = e^{+i\pi} z$ requires equation (45) with the lower sign

$$\Delta E_n(z) = E_n(e^{-i\pi} z) - E_n(e^{+i\pi} z) \quad (56)$$

$$\sim [1 - \exp(\Delta w_+(n, z) \partial / \partial n)] E_n^{\text{RS}}(-z) \quad (57)$$

$$= -\lambda \Delta w_+ \frac{\partial}{\partial n} E_n^{\text{RS}}(-z) - \lambda^2 \frac{1}{2} (\Delta w_+)^2 \frac{\partial^2}{\partial n^2} E_n^{\text{RS}}(-z) + \dots \quad (58)$$

$$= -\lambda \Delta w_+^{(1)} \frac{\partial}{\partial n} E_n^{\text{RS}}(-z) - \lambda^2 \left[\Delta w_+^{(2)} \frac{\partial}{\partial n} E_n^{\text{RS}}(-z) + \frac{1}{2} (\Delta w_+^{(1)})^2 \frac{\partial^2}{\partial n^2} E_n^{\text{RS}}(-z) \right] + O(\lambda^3). \quad (59)$$

Putting the two results together, we find that the first exponentially small correction to the energy $\Delta E_n^{(1)}(z)$ and the second exponentially small correction to the energy $\Delta E_n^{(2)}(z)$ are given respectively by

$$\Delta E_n^{(1)}(z) = \pm \Delta w_{\mp}^{(1)} \frac{\partial E_n^{\text{RS}}(-z)}{\partial n} \quad (60)$$

$$= -iB(n, z) f(n, z) \frac{\partial E_n^{\text{RS}}(-z)}{\partial n} \quad (61)$$

$$\Delta E_n^{(2)}(z) = \pm \Delta w_{\mp}^{(2)} \frac{\partial E_n^{\text{RS}}(-z)}{\partial n} \pm \frac{1}{2} [\Delta w_{\mp}^{(1)}]^2 \frac{\partial^2 E_n^{\text{RS}}(-z)}{\partial n^2} \quad (62)$$

$$= i \frac{\pi}{2} B(n, z)^2 f(n, z)^2 \frac{\partial E_n^{\text{RS}}(-z)}{\partial n} \pm B(n, z)^2 \frac{\partial E_n^{\text{RS}}(-z)}{\partial n} \left\{ f(n, z)^2 \left[\ln \left(\frac{z}{4} \right) + \psi(n+1) \right] - f(n, z) \frac{\partial f(n, z)}{\partial n} \right\} \mp \frac{1}{2} B(n, z)^2 f(n, z)^2 \frac{\partial^2 E_n^{\text{RS}}(-z)}{\partial n^2} \quad (g = e^{\mp i\pi} z \quad \arg z = \mp \epsilon \quad \epsilon > 0). \quad (63)$$

Note that the expansion $\Delta E_n^{(1)}(z)$ is the same, independent of the sign of $\arg z$. Moreover it is formally purely imaginary when z is real and positive. It is of the form $-iB(n, z)$ times a power series in z with constant term $b_n^{(0)} = 1$,

$$\Delta E_n^{(1)}(z) = -iB(n, z) \sum_{k=0}^{\infty} b_n^{(k)} (3z)^k. \quad (64)$$

Furthermore, equation (61) provides a direct way to evaluate the coefficients $b_n^{(k)}$.

The second exponentially small contribution has both a formally real and a formally imaginary part, which we denote by

$$\Delta E_n^{[2]} = \Delta E_n^{[2,r]} + i\Delta E_n^{[2,i]}. \tag{65}$$

The first term of equation (63) is a formula for $i\Delta E_n^{[2,i]}(z)$ that is of the form $i\pi/2$ times $B(n, z)^2$ times a power series in z with constant term $c_n^{(0)} = 1$,

$$i\Delta E_n^{[2,i]}(z) = i\frac{\pi}{2} \left[2\pi C_n(3z)^{-n-\frac{1}{2}} e^{-\frac{1}{3z}} \right]^2 \sum_{l=0}^{\infty} c_n^{(l)}(3z)^l. \tag{66}$$

The remaining two terms in equation (63) give $\Delta E_n^{[2,r]}(z)$. Note the (\pm) sign explicit in $\Delta E_n^{[2,r]}$: as $\text{Im } z$ passes through 0, the asymptotic expansion $\Delta E_n^{[2,r]}(z)$ has a discontinuous change in sign:

$$\Delta E_n^{[2,r]}(z - i0) = -\Delta E_n^{[2,r]}(z + i0) \quad (z > 0). \tag{67}$$

Except for the sign, the expansions on either side of the real axis are otherwise formally identical. To avoid sign confusion that could arise when $\Delta E_n^{[2,r]}(z \pm i0)$ might appear in a dispersion relation, we introduce a symbol to denote an expansion that is *formally continuous* across the real axis, that coincides with $\Delta E_n^{[2,r]}(z)$ when $\text{Im } z < 0$, but that is $-\Delta E_n^{[2,r]}(z)$ when $\text{Im } z > 0$:

$$\Delta E_n^{[2,r,-]}(z) \equiv \Delta E_n^{[2,r]}(z) \quad (\text{Im } z < 0) \tag{68}$$

$$\equiv -\Delta E_n^{[2,r]}(z) \quad (\text{Im } z > 0). \tag{69}$$

The upper sign in equation (63) leads to a formula for the $\Delta E_n^{[2,r,-]}$:

$$\begin{aligned} \Delta E_n^{[2,r,-]}(z) &= B(n, z)^2 \frac{\partial E_n^{\text{RS}}(-z)}{\partial n} \left\{ f(n, z)^2 \left[\ln\left(\frac{z}{4}\right) + \psi(n+1) \right] - f(n, z) \frac{\partial f(n, z)}{\partial n} \right\} \\ &\quad - \frac{1}{2} B(n, z)^2 f(n, z)^2 \frac{\partial^2 E_n^{\text{RS}}(-z)}{\partial n^2} \end{aligned} \tag{70}$$

$$= B(n, z)^2 \left\{ \left[\ln\left(\frac{z}{4}\right) + \psi(n+1) \right] \sum_{l=0}^{\infty} c_n^{(l)}(3z)^l - \frac{1}{2} \sum_{l=1}^{\infty} d_n^{(l)}(3z)^l \right\}. \tag{71}$$

Once the function $f(n, z)$ has been given, equations (61) and (63) specify the energy discontinuity through second-exponentially-small order.

2.7. Comment on signs of $\Delta E_n^{[k,r]}(z)$ and $\Delta E_n^{[k,i]}(z)$

From equations (40)–(45) one can see that Δw_- and Δw_+ enjoy a conjugate relationship: for real g' , and with $z = g' e^{\pm i\epsilon}$

$$\Delta w_{\pm}(n, z) = [\Delta w_{\mp}(n, z^*)]^* \tag{72}$$

$$\Delta w_{\pm}(n, g' e^{\pm i\epsilon}) = [\Delta w_{\mp}(n, g' e^{\mp i\epsilon})]^*. \tag{73}$$

Via equations (53) and (57) this implies a conjugate relationship between the expansions for $\Delta E_n(z)$,

$$\Delta E_n(g' e^{i\epsilon}) \sim [1 - \exp(\Delta w_+(n, g' e^{i\epsilon}) \partial / \partial n)] E_n^{\text{RS}}(-g' e^{i\epsilon}) \quad (74)$$

$$= -[\exp(\Delta w_-(n, g' e^{-i\epsilon}) \partial / \partial n) - 1]^* E_n^{\text{RS}}(-g' e^{-i\epsilon})^* \quad (75)$$

$$\sim -\Delta E_n(g' e^{-i\epsilon})^*. \quad (76)$$

In particular, since by definition $\Delta E_n^{\{k,r\}}(z)$ and $\Delta E_n^{\{k,i\}}(z)$ are formally real expansions for real z , it follows that

$$\Delta E_n^{\{k\}}(g' e^{i\epsilon}) = -\Delta E_n^{\{k\}}(g' e^{-i\epsilon})^* \quad (77)$$

$$\Delta E_n^{\{k,r\}}(g' e^{i\epsilon}) = -\Delta E_n^{\{k,r\}}(g' e^{-i\epsilon})^* \quad (78)$$

$$\Delta E_n^{\{k,i\}}(g' e^{i\epsilon}) = +\Delta E_n^{\{k,i\}}(g' e^{-i\epsilon})^* \quad (79)$$

and the formally imaginary terms in $\Delta E_n^{\{k\}}$ will remain unchanged, while the formally real terms will change sign. That is, the sign of the formally real terms is discontinuous across the real axis.

3. Evaluation of the power series for $f(n, z)$

The logarithm of $f(n, z)$ is simpler than $f(n, z)$ in that the coefficient of z^k is a polynomial in n of only degree $k + 1$ rather than $2k$

$$\ln f(n, z) = -z \left(\frac{59}{24} + \frac{17}{4}n + \frac{17}{4}n^2 \right) - z^2 \left(\frac{347}{32} + \frac{59}{2}n + \frac{375}{16}n^2 + \frac{125}{8}n^3 \right) + O(z^3). \quad (80)$$

Comparing equation (80) for $\ln f(n, z)$ with equations (17)–(20) for the RS expansion, one notices a remarkable connection,

$$\ln f(n, z) = \frac{1}{3} \frac{d}{dn} E_n^{(2)} z - \frac{1}{6} \frac{d}{dn} E_n^{(3)} z^2 + O(z^3). \quad (81)$$

We have verified through degree $N = 10$ in z that (cf [9])

$$\ln f(n, z) = \sum_{k=1}^N z^k \frac{1}{3k} (-1)^{k+1} \frac{d}{dn} E_n^{(k+1)} + O(z^{N+1}). \quad (82)$$

Since the RS coefficients $E_n^{(k+1)}$ are far easier to calculate (in terms of computer memory and time) than the series for $f(n, z)$ directly, we have used equation (82) with $N = 50$ to calculate the corresponding terms of $\ln f(n, z)$ indirectly.

We remark that all information about $E_n(g)$ is necessarily contained in the RS energy coefficients, because the RS series is Borel summable to $E_n(g)$. That there exists a recipe to obtain the $\ln f(n, z)$ coefficients from the RS coefficients is therefore not unexpected—but why the recipe is so simple is not obvious.

4. Evaluation of the expansion coefficients $b_n^{(k)}$, $c_n^{(k)}$ and $d_n^{(k)}$

An explicit formula for the expansion coefficients $b_n^{(k)}$ for $\Delta E_n^{\{1\}}$ follows from equations (61) and (64):

$$\sum_{k=0}^{\infty} b_n^{(k)} (3z)^k = f(n, z) \frac{\partial E_n^{\text{RS}}(-z)}{\partial n}. \quad (83)$$

Explicit formulae for the expansion coefficients $c_n^{(k)}$ and $d_n^{(k)}$ for $\Delta E_n^{\{2\}}$ follow from equations (63), (66), and (71):

Table 1. The coefficients $b_n^{(k)}$.

k	$b_n^{(k)}$
0	1
1	$-\frac{95}{72} - \frac{29}{12}n - \frac{17}{12}n^2$
2	$-\frac{13\,259}{10\,368} - \frac{1733}{864}n + \frac{29}{108}n^2 + \frac{27}{16}n^3 + \frac{289}{288}n^4$
3	$-\frac{8956\,043}{2239\,488} - \frac{1083\,329}{124\,416}n - \frac{635\,915}{124\,416}n^2 + \frac{1391}{864}n^3 + \frac{3923}{2304}n^4 + \frac{119}{3456}n^5 - \frac{4913}{10\,368}n^6$

Table 2. The coefficients $c_n^{(k)}$.

k	$c_n^{(k)}$
0	1
1	$-\frac{77}{36} - \frac{23}{6}n - \frac{17}{6}n^2$
2	$-\frac{2765}{2592} - \frac{59}{216}n + \frac{1357}{216}n^2 + \frac{133}{18}n^3 + \frac{289}{72}n^4$
3	$-\frac{1259\,693}{279\,936} - \frac{105\,125}{15\,552}n - \frac{4961}{15\,552}n^2 + \frac{9275}{1296}n^3 - \frac{25}{9}n^4 - \frac{799}{144}n^5 - \frac{4913}{1296}n^6$

Table 3. The coefficients $d_n^{(k)}$.

k	$d_n^{(k)}$
0	0
1	$-\frac{23}{6} - \frac{17}{3}n$
2	$-\frac{59}{216} + \frac{1357}{108}n + \frac{133}{6}n^2 + \frac{289}{18}n^3$
3	$-\frac{105\,125}{15\,552} - \frac{4961}{7776}n + \frac{9275}{432}n^2 - \frac{100}{9}n^3 - \frac{3995}{144}n^4 - \frac{4913}{216}n^5$

$$\sum_{k=0}^{\infty} c_n^{(k)} (3z)^k = f(n, z)^2 \frac{\partial E_n^{\text{RS}}(-z)}{\partial n} \tag{84}$$

$$\sum_{k=1}^{\infty} d_n^{(k)} (3z)^k = 2f(n, z) \frac{\partial f(n, z)}{\partial n} \frac{\partial E_n^{\text{RS}}(-z)}{\partial n} + f(n, z)^2 \frac{\partial^2 E_n^{\text{RS}}(-z)}{\partial n^2} \tag{85}$$

$$= \frac{\partial}{\partial n} \sum_{k=0}^{\infty} c_n^{(k)} (3z)^k. \tag{86}$$

Equation (86), which is an immediate consequence of equation (85), shows further that the $d_n^{(k)}$ are just the derivatives of the $c_n^{(k)}$ with respect to n . The practical evaluation of $b_n^{(k)}$, $c_n^{(k)}$ and $d_n^{(k)}$ is based on equation (82) for $\ln f(n, z)$. First, the RS expansion for the $E_n^{(k)}$ is carried out in such a way to obtain the $E_n^{(k)}$ as polynomials (of degree $k + 1$) in n . Second, $f(n, z)$ is obtained via exponentiation of equation (82). The rest follows from equations (83), (84) and (86). Tables 1–3 contain the first few coefficients as explicit functions of n .

4.1. Asymptotic forms for $E_n^{(k)}$, $b_n^{(k)}$, $c_n^{(k)}$ and $d_n^{(k)}$

It is important to know the leading asymptotic behaviour of $E_n^{(k)}$, $b_n^{(k)}$, $c_n^{(k)}$ and $d_n^{(k)}$ with respect to k , which is required to estimate the optimum truncation of the hyperasymptotic series obtained in [2].

First note that the leading asymptotic term of the RS coefficient is [8]

$$E_n^{(k)} \sim -C_n (-3)^k \Gamma\left(k + n + \frac{1}{2}\right) [1 + O(k^{-1})] \quad (87)$$

whence

$$\frac{\partial E_n^{(k)}}{\partial n} = -C_n (-3)^k \Gamma\left(k + n + \frac{1}{2}\right) \left[\ln\left(k + n + \frac{1}{2}\right) + \ln 12 - \psi(n + 1) + O(k^{-1} \ln k) \right]. \quad (88)$$

From equations (82) and (83), one has

$$\sum_{k=0}^{\infty} b_n^{(k)} (3z)^k \sim \frac{\partial E_n^{\text{RS}}(-z)}{\partial n} \exp \left[\sum_{l=1}^{\infty} (-1)^{l+1} \frac{z^l}{3l} \frac{dE_n^{(l+1)}}{dn} \right] \quad (89)$$

from which it follows that

$$b_n^{(k)} = -2C_n \Gamma\left(k + n + \frac{1}{2}\right) \left[\ln\left(k + n + \frac{1}{2}\right) + \ln 12 - \psi(n + 1) + O(k^{-1} \ln k) \right] \quad (90)$$

$$c_n^{(k)} = -3C_n \Gamma\left(k + n + \frac{1}{2}\right) \left[\ln\left(k + n + \frac{1}{2}\right) + \ln 12 - \psi(n + 1) + O(k^{-1} \ln k) \right] \quad (91)$$

$$d_n^{(k)} = -3C_n \Gamma\left(k + n + \frac{1}{2}\right) \left\{ \left[\ln\left(k + n + \frac{1}{2}\right) + \ln 12 - \psi(n + 1) \right]^2 + O(k^{-1} (\ln k)^2) \right\}. \quad (92)$$

Equations (87) and (90)–(92) have been put in as similar form as possible by exploiting the flexibility of the $O(k^{-1} \ln k)$. The 3:2 asymptotic ratio of $c_n^{(k)}$ to $b_n^{(k)}$ is apparent in tables 4 and 5.

5. Summary

In the companion paper [2] we discuss the derivation of higher-level dispersion relations for the quartic anharmonic oscillator. These dispersion relations are driven by the purely imaginary discontinuity of the energy across the negative coupling-constant axis, and in this paper we have calculated explicitly up to second-exponentially-small order the asymptotic expansion of this discontinuity.

The main steps of the derivation are given in section 2. The first step is to match asymptotic wavefunctions based on the Whittaker confluent hypergeometric function at the origin and on the Airy function near the outer turning point. Matching on the ‘first sheet’ of the coupling constant complex plane yields the Borel-summable RS series. Matching on the ‘second sheet’ gives the RS series with a small shift in the oscillator quantum number as it enters the formulae for the RS coefficients. This shift Δw satisfies equation (40), obtained from the match, and it can be found iteratively as the sum of successively exponentially smaller subseries (equations (46)–(51)). The second step is to plug these formulae for Δw into the ‘shifted’ RS series to obtain formulae for $\Delta E_n^{(1)}(z)$ and $\Delta E_n^{(2)}(z)$ (equations (61) and (63)). The resulting asymptotic expansion for $\Delta E_n^{(1)}(z)$ is formally purely imaginary for z real. The asymptotic expansion for $\Delta E_n^{(2)}(z)$ contains formally real series, as well as imaginary, but the sign of the formally real terms changes discontinuously on the positive real z axis, an interesting and essential fact. Explicit recipes for the coefficients $b_n^{(k)}$, $c_n^{(k)}$ and $d_n^{(k)}$ that enter these series are given in section 4 after evaluation of $f(n, z)$ in section 3.

Table 4. Coefficients $E_0^{(k)}$, $b_0^{(k)}$, $c_0^{(k)}$ and $d_0^{(k)}$ for the $n = 0$ ground state.

k	$(-1)^{k+1} E_0^{(k)}$	$-b_0^{(k)}$	$-c_0^{(k)}$	$-d_0^{(k)}$
0	-0.5	-1.0	-1.0	0.0
1	0.75	1.319 444	2.138 889	3.833 333
2	2.625	1.278 839	1.066 744	0.273 148
3	$2.081\,25 \times 10^1$	3.999 148	4.499 932	6.759 581
4	$2.412\,891 \times 10^2$	$1.780\,162 \times 10^1$	$2.091\,950 \times 10^1$	$5.021\,742 \times 10^1$
5	$3.580\,980 \times 10^3$	$9.864\,511 \times 10^1$	$1.224\,627 \times 10^2$	$3.372\,231 \times 10^2$
6	$6.398\,281 \times 10^4$	$6.437\,460 \times 10^2$	$8.175\,298 \times 10^2$	$2.654\,708 \times 10^3$
7	$1.329\,734 \times 10^6$	$4.803\,501 \times 10^3$	$6.273\,846 \times 10^3$	$2.211\,347 \times 10^4$
8	$3.144\,821 \times 10^7$	$4.024\,606 \times 10^4$	$5.334\,306 \times 10^4$	$2.060\,674 \times 10^5$
9	$8.335\,416 \times 10^8$	$3.739\,607 \times 10^5$	$5.043\,387 \times 10^5$	$2.054\,751 \times 10^6$
10	$2.447\,894 \times 10^{10}$	$3.818\,256 \times 10^6$	$5.200\,175 \times 10^6$	$2.246\,345 \times 10^7$
\vdots	\vdots	\vdots	\vdots	\vdots
45	$2.240\,859 \times 10^{76}$	$1.015\,741 \times 10^{56}$	$1.495\,963 \times 10^{56}$	$9.719\,427 \times 10^{56}$
46	$3.060\,931 \times 10^{78}$	$4.642\,470 \times 10^{57}$	$6.838\,813 \times 10^{57}$	$4.463\,606 \times 10^{58}$
47	$4.272\,878 \times 10^{80}$	$2.168\,189 \times 10^{59}$	$3.195\,840 \times 10^{59}$	$2.092\,655 \times 10^{60}$
48	$6.092\,777 \times 10^{82}$	$1.034\,259 \times 10^{61}$	$1.524\,755 \times 10^{61}$	$1.002\,742 \times 10^{62}$
49	$8.870\,460 \times 10^{84}$	$5.036\,817 \times 10^{62}$	$7.429\,586 \times 10^{62}$	$4.901\,004 \times 10^{63}$
50	$1.318\,042 \times 10^{87}$	$2.503\,201 \times 10^{64}$	$3.692\,988 \times 10^{64}$	$2.446\,113 \times 10^{65}$

Table 5. Coefficients $E_1^{(k)}$, $b_1^{(k)}$, $c_1^{(k)}$ and $d_1^{(k)}$ for the $n = 1$ first excited state.

k	$(-1)^{k+1} E_1^{(k)}$	$-b_1^{(k)}$	$-c_1^{(k)}$	$-d_1^{(k)}$
0	-1.5	-1.0	-1.0	0.0
1	3.75	5.152 778	8.805 556	9.5
2	$-2.062\,5 \times 10^1$	0.325 135	$-1.634\,529 \times 10^1$	$-5.051\,388\,9 \times 10^1$
3	$2.446\,875 \times 10^2$	$1.494\,444 \times 10^1$	$1.653\,916 \times 10^1$	$4.752\,720 \times 10^1$
4	$4.066\,289 \times 10^3$	$1.142\,670 \times 10^2$	$8.098\,048 \times 10^1$	$5.329\,175 \times 10^1$
5	$8.322\,064 \times 10^4$	$9.663\,260 \times 10^2$	$7.633\,385 \times 10^2$	$8.550\,329 \times 10^2$
6	$1.979\,440 \times 10^6$	$9.045\,594 \times 10^3$	$7.738\,320 \times 10^3$	$1.166\,120 \times 10^4$
7	$5.302\,892 \times 10^7$	$9.249\,919 \times 10^4$	$8.409\,585 \times 10^4$	$1.556\,337 \times 10^5$
8	$1.570\,097 \times 10^9$	$1.022\,762 \times 10^6$	$9.763\,672 \times 10^5$	$2.106\,882 \times 10^6$
9	$5.075\,057 \times 10^{10}$	$1.213\,969 \times 10^7$	$1.206\,855 \times 10^7$	$2.937\,931 \times 10^7$
10	$1.775\,710 \times 10^{12}$	$1.538\,884 \times 10^8$	$1.583\,563 \times 10^8$	$4.250\,134 \times 10^8$
\vdots	\vdots	\vdots	\vdots	\vdots
45	$1.118\,461 \times 10^{79}$	$4.022\,325 \times 10^{58}$	$5.550\,160 \times 10^{58}$	$3.026\,516 \times 10^{59}$
46	$1.564\,577 \times 10^{81}$	$1.886\,953 \times 10^{60}$	$2.608\,567 \times 10^{60}$	$1.430\,122 \times 10^{61}$
47	$2.235\,423 \times 10^{83}$	$9.039\,524 \times 10^{61}$	$1.251\,882 \times 10^{62}$	$6.899\,112 \times 10^{62}$
48	$3.260\,770 \times 10^{85}$	$4.420\,245 \times 10^{63}$	$6.132\,083 \times 10^{63}$	$3.396\,451 \times 10^{64}$
49	$4.853\,967 \times 10^{87}$	$2.205\,396 \times 10^{65}$	$3.064\,509 \times 10^{65}$	$1.705\,686 \times 10^{66}$
50	$7.370\,811 \times 10^{89}$	$1.122\,267 \times 10^{67}$	$1.561\,902 \times 10^{67}$	$8.734\,727 \times 10^{67}$

The function $f(n, z)$, the first few terms of which are given by equation (80), is a power series in z whose coefficients are polynomials in n that arise from the match of the Whittaker and Airy-based solutions. Its extraction is complicated. That $\ln f(n, z)$ has such a simple

relationship to the derivative of the RS series (see equation (82)) is both remarkable and what made possible our calculation of the $b_n^{(k)}$, $c_n^{(k)}$ and $d_n^{(k)}$ coefficients to high order.

These results for $b_n^{(k)}$, $c_n^{(k)}$ and $d_n^{(k)}$ are used in the companion paper [2] to exemplify how hyperasymptotics can be applied to derive exponentially improved asymptotic approximations to the eigenvalues of oscillator systems.

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