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On the $\alpha x^2 + \beta x^4$ interaction

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Abstract. By applying the Laplace transform method we obtain a class of exact solutions for the Schrödinger equation with the potential $V(x) = \alpha x^2 + \beta x^4$, $x > 0$, $\alpha \geqslant 0$, $\beta < 0$, the corresponding energy spectrum being continuous. A particular feature of these eigensolutions is that they may not be accessible to perturbation theory. The properties of the solutions obtained are investigated and their relation to the case where $x \leqslant 0$ is included is discussed.

1. Introduction

In this paper we consider the problem of the anharmonic oscillator with quartic anharmonicity. Interest in such a model stems mainly from the fact that, as remarked by Simon (1970), the perturbation x^4 is singular. Now, singular perturbations are not uncommon in physics, for instance in the Born–Oppenheimer approximation in solid or molecular physics, where we have to take account of corrections which are singular perturbations in nature, or in quantum field theory, where one has a singular interaction Hamiltonian. Moreover, the above oscillator corresponds to a field theory (Bender and Wu 1969) in zero space dimensions for which the perturbation series diverges (Simon 1970).

The foregoing examples indicate that it may be worthwhile to study the properties of singular perturbations, in our case of x^4, as such an investigation may reveal inherent physical phenomena. Since the work of Bender and Wu (1969) and the comprehensive contribution of Simon on the interaction

$$V_1(x) = \alpha x^2 + \beta x^4, \qquad -\infty < x < \infty, \tag{1.1}$$

where $\alpha > 0$ and β is allowed to assume complex values, a lot of work (Haan and Mütte 1979, Halliday and Surenyi 1980, Hioe *et al* 1978, Mathews *et al* 1981) has been done on the calculation of energy levels of the potential in equation (1.1) by application of perturbational and numerical methods. However, it may be desirable to obtain for the interaction (1.1) exact results since they can serve as a testing ground for the various approximate approaches. This may be all the more important, as it has been recently proved (Khare 1981) that rigorous solutions and eigenvalues for anharmonic oscillators (Flessas and Das 1980, Flessas and Watt 1981) may not be accessible to conventional perturbation theory. Now, the interaction (1.1) possesses the following striking characteristic. All the methods which yield exact solutions of

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the Schrödinger equation for more general than (1.1) polynomial or even non-polynomial interactions (Flessas and Das 1980, Flessas 1981a, b, Flessas and Watt 1981, Whitehead *et al* 1982, Znojil 1982) fail when applied to (1.1). Motivated by this feature, which may be construed as a manifestation of the singular character of the x^4 perturbation, and by some recent work (Flessas 1982), we consider $\alpha x^2 \mp \beta x^4$ on the half axis $x>0$. As a result we have constructed rigorous eigensolutions for the case $x>0$ provided $\beta=|\beta|\exp(\mathrm{i}\pi)$ or $\beta=|\beta|\exp(3\pi\mathrm{i}/2)$. These solutions are valid for $\alpha \geqslant 0$ and it will be seen that they most probably cannot be obtained by standard perturbation theory.

In § 2 we present our results in the form of a theorem and carry out the proof, while in § 3 we discuss the solutions obtained and their relevance to the interaction (1.1). In appendices 1 and 2 we have included some mathematical details.

2. Eigenfunctions and the energy spectrum

In this section we shall prove the following theorem.

Theorem 2.1. The Schrödinger equation

$$y''(x)+[E-V(x)]y(x)=0 \tag{2.1}$$

where

$$V(x)=\begin{cases}\alpha x^2+\beta x^4, & x_1\leqslant x\leqslant x_2,\ x_1>0,\ x_2>(\alpha/|\beta|^{1/2}),\ \alpha\geqslant 0, \quad (2.2)\\ V_0, & -\infty<x\leqslant x_1, \qquad V_0>0, \quad (2.3)\\ V_0', & x_2\leqslant x<\infty, \qquad V_0'<0, \quad (2.4)\end{cases}$$

is satisfied by

$$y_1(x)=\exp\left[\mathrm{i}\left(\frac{\alpha}{(4|\beta|)^{1/2}}x-\left(\frac{|\beta|}{9}\right)^{1/2}x^3\right)\right]\int_0^\infty \exp(-sx)f(s)\,\mathrm{d}s,$$

$$0<x_1\leqslant x\leqslant x_2, \tag{2.5}$$

$$y(x)=\begin{cases}=A\exp[\mathrm{i}(E-V_0)^{1/2}x]+B\exp[-\mathrm{i}(E-V_0)^{1/2}x], & -\infty<x\leqslant x_1, \quad (2.6)\\ =A'\exp[\mathrm{i}(E-V_0')^{1/2}x]+B'\exp[-\mathrm{i}(E-V_0')^{1/2}x], & x_2\leqslant x<\infty, \quad (2.7)\end{cases}$$

where A, B and A', B' are determined from the usual continuity conditions at x_1 and x_2, respectively,

$$f(s)=\sum_{n=0}^{\infty}c_n s^n, \qquad c_0\neq 0, \tag{2.8}$$

convergent for $s\in[0,\infty)$, and

$$\mathrm{i}^3(4|\beta|)^{1/2}(n+1)^2c_{n+1}-\left(\frac{\mathrm{i}^2\alpha^2}{4|\beta|}+E\right)c_n+\frac{2\mathrm{i}\alpha}{(4|\beta|)^{1/2}}c_{n-1}-c_{n-2}=0$$

$$c_{-1}=c_{-2}=0, \qquad n=0,1,2,\ldots. \tag{2.9}$$

The energy, E, spectrum is continuous and comprises all finite numbers satisfying $E\geqslant V_0$.

Proof. We have

$$y''(x)+(E-\alpha x^2-\beta x^4)y(x)=0, \qquad 0<x_1\leqslant x\leqslant x_2. \tag{2.10}$$

Previous results (Simon 1970, Flessas and Watt 1981) suggest that the ansatz

$$y(x)=\exp[(ax+bx^3)]g(x), \tag{2.11}$$

a, b being constants which have yet to be specified, is a suitable one. Inserting (2.11) into (2.10) and letting a, b be defined by

$$9b^2=\beta, \qquad 6ab=\alpha, \tag{2.12}$$

we obtain

$$g''(x)+(2a+6bx^2)g'(x)+(a^2+E+6bx)g(x)=0, \qquad 0<x_1\leqslant x\leqslant x_2. \tag{2.13}$$

We write $g(x)$ as the Laplace transform of a function $f(s)$. Thus

$$g(x)=\int_0^\infty \exp(-sx)f(s)\,\mathrm{d}s, \qquad 0<x_1\leqslant x\leqslant x_2, \tag{2.14}$$

and assuming that the integral exists (this is justified later), we can build $g'(x)$, $g''(x)$. Then we deduce that (2.14) is a solution to (2.13) provided that the following two relations hold:

$$I(\infty)-I(0)=0, \qquad I(s)=6b\exp(-sx)[sxf(s)+sf'(s)], \tag{2.15}$$

$$6bsf''(s)+6bf'(s)+[-s^2+2as-(a^2+E)]f(s)=0. \tag{2.16}$$

We first turn our attention to the differential equation (2.16). From the indicial equation of (2.16) it follows that we can write

$$f(s)=\sum_{n=0}^{\infty} c_n s^n, \qquad c_0\neq 0. \tag{2.17}$$

According to the general theory of differential equations (Morse and Feshbach 1953), the power series in (2.17) converges for $0\leqslant s<\infty$, as the only singularities of (2.16) are at $s=0$ and $s=\infty$. We note in passing that from the convergence of the series in (2.17) for $s\in[0,\infty)$ it readily follows that both $|c_n|\to_{n\to\infty}0$ and $[|c_n/c_{n-1}|]\to_{n\to\infty}0$. The c's fulfil

$$6b(n+1)^2c_{n+1}-(a^2+E)c_n+2ac_{n-1}-c_{n-2}=0, \qquad c_{-1}=c_{-2}=0,$$
$$n=0,1,2,\ldots. \tag{2.18}$$

Using (2.18), it is straightforward to deduce a closed form for c_n with $c_1=c_0(a^2+E)/(6b1^2)$:

$$c_n=\frac{c_0}{(6b)^n(n!)^2}\begin{vmatrix} a^2+E & 6b1^2 & & 0 & 0 & 0 & \cdots & \\ 2a & a^2+E & 6b2^2 & 0 & 0 & 0 & \cdots & \\ 1 & 2a & a^2+E & 6b3^2 & 0 & 0 & \cdots & \\ 0 & 1 & 2a & a^2+E & 6b4^2 & 0 & \cdots & \\ 0 & 0 & 1 & 2a & a^2+E & 6b5^2 & \cdots & \\ \vdots & \vdots & \vdots & \vdots & & & \ddots & \\ & & & & & \ddots & a^2+E & 6b(n-1)^2 \\ & & & & & & 2a & a^2+E \end{vmatrix},$$

$$n\geqslant 2. \tag{2.19}$$

In what follows we investigate the behaviour of $f(s)$ for $s \gg 1$. To this end we observe that (2.18) yields for every *finite E*

$$c_{n+1}/c_n = 1/(6b)^{1/3} n^{2/3}, \qquad n \gg 1. \tag{2.20}$$

Henceforward we assume that $\beta = -|\beta| < 0$. Then by virtue of (2.12)

$$\frac{c_{n+1}}{c_n} = -\frac{\mathrm{i}L}{n^{2/3}}, \qquad L = (4|\beta|)^{-1/6} > 0, \qquad n \gg 1. \tag{2.21}$$

In the β plane we have, in fact, $\beta = \mathrm{e}^{\mathrm{i}\pi}|\beta|$. Hence (2.12) gives $(6b)^{1/3} = (4|\beta|)^{1/6} \exp[\mathrm{i}(\pi/6 + k\, 2\pi/6)]$ with $k = 0, 1, \ldots, 5$. Equation (2.21) exhibits the $k = 1$ case, the $k = 4$ case differing only in the (inessential for our purposes) sign of i. The remaining k-values give rise to relations similar to (2.21) and can be treated along the lines of theorem 2.1.

Now, equation (2.21) implies that $f(s)$ for $s \gg 1$ behaves like

$$\begin{aligned} F(s) &= \sum_{n=0}^{\infty} (-\mathrm{i})^n \frac{z_1^n}{(n!)^{2/3}} \\ &= \sum_{n=0}^{\infty} (-1)^n \frac{z^n}{[(2n)!]^{2/3}} + \frac{\mathrm{i}}{z_1} \sum_{n=1}^{\infty} (-1)^n \frac{z^n}{[(2n-1)!]^{2/3}} \\ &= \sum\nolimits_1 + \frac{\mathrm{i}}{z_1} \sum\nolimits_2, \qquad z = z_1^2, \qquad z_1 = Ls, \end{aligned} \tag{2.22}$$

the meaning of Σ_1 and Σ_2 being obvious. In the following we compare Σ_1 with

$$\exp(-z) = \sum_{n=0}^{\infty} (-1)^n \frac{z^n}{n!}. \tag{2.23}$$

By applying a result from the theory of analytic continuation (Morse and Feshbach 1953), we can deduce

$$\sum\nolimits_1 = \exp(-z) \sum_{n=0}^{\infty} S_n \frac{z^n}{n!} = \exp(-z) \sum\nolimits_1', \tag{2.24}$$

$$S_n = \sum_{k=0}^{n} (-1)^k \binom{n}{k} \frac{k!}{[(2k)!]^{2/3}}. \tag{2.25}$$

In appendix 1 we shall prove that

$$|S_n| < n, \qquad n = 1, 2, 3, \ldots. \tag{2.26}$$

On combining (2.24)–(2.26), we get

$$\left|\sum\nolimits_1'\right| < 1 + \sum_{n=1}^{\infty} \frac{z^n}{(n-1)!} < 1 + \sum_{n=1}^{\infty} \frac{(n+1)}{n!} z^n = \exp(z)(1+z), \tag{2.27}$$

the second inequality in (2.27) following from $1/(n-1)! < (n+1)/n!$. Consequently (2.24) shows

$$\left|\sum\nolimits_1\right| = \exp(-z)\left|\sum\nolimits_1'\right| < 1 + z. \tag{2.28}$$

Furthermore, since

$$((2n)!/(2n+2)!)^{2/3} = ((2n-1)!/(2n+1)!)^{2/3}, \qquad n \gg 1, \tag{2.29}$$

Σ_2 in (2.22) has the same asymptotic behaviour for $s \gg 1$ as Σ_1. Hence, as (2.28) shows, and recalling $z=(Ls)^2$, $F(s)$ and thus also $f(s)$ cannot behave for $s \gg 1$ more strongly than

$$\pm(1+L^2s^2)+(\mathrm{i}/Ls)(\pm(1+L^2s^2)). \tag{2.30}$$

Therefore the integral in (2.14) exists and obviously (2.15) is automatically satisfied. Equation (2.9) is simply (2.18), where we have used (2.12) and the choice of β made in (2.21). On combining (2.11)–(2.12) and (2.14), we can establish the truth of (2.5). As (2.6)–(2.7) are trivial we need only note that for $x \to \pm\infty$, $y(x)$ must remain bounded. Thus we obtain $E \geqslant V_0$, and, therefore, since the basic relation (2.20) holds for any finite E, the last part of the theorem is verified. The continuous spectrum thus obtained, which may give rise to tunnelling effects not considered here, might have been expected in view of the structure of $V(x)$ for $x \leqslant x_1$ and $x \geqslant x_2$ as given by (2.3)–(2.4), and it does not preclude the existence of discrete E-levels. The important thing is that the exact solutions pertaining to that spectrum do not seem, as will be verified in § 3, to be obtainable otherwise than as in the theorem.

We wish to point out that theorem 2.1 is valid also for $\beta=|\beta|\exp(3\pi\mathrm{i}/2)$. In such a case (2.22) is replaced by

$$\sum_{n=0}^{\infty}(-1)^n\cos\left(\frac{\pi}{4}n\right)\frac{z^n}{(n!)^{2/3}}-\mathrm{i}\sum_{n=1}^{\infty}(-1)^n\sin\left(\frac{\pi}{4}n\right)\frac{z^n}{(n!)^{2/3}}, \tag{2.31}$$

which, as some thought reveals, behaves for $s \gg 1$ at the most as L^6s^6. Consequently, the above procedure applies here and we arrive at the equations equivalent to (2.5)–(2.9) with the appropriate coefficients for x and x^3 in (2.5) and a corresponding modification of the c's in (2.9). Moreover, the theorem clearly holds for any $x_2>x_1>0$ and arbitrary real V_0, V_0'. The choice concerning x_2, V_0 and V_0' in (2.2)–(2.4) facilitates the discussion in § 3.

3. Discussion of the solutions

Let us first examine (2.14). On using (2.17) and integrating, we easily deduce

$$g(x)=\sum_{n=0}^{\infty}\frac{n!}{x^{n+1}}c_n, \qquad 0<x_1\leqslant x\leqslant x_2<\infty. \tag{3.1}$$

Now the c_n for $n \gg 1$ behave like $1/(n!)^{2/3}$, as (2.20) shows. Thus, if the series in (3.1) converged for some finite x, we should have

$$((n!/x^{n+1})c_n)\to 0, \qquad n\to\infty, \qquad 0<x_1\leqslant x\leqslant x_2<\infty, \tag{3.2}$$

which is impossible due to the behaviour of c_n for $n \gg 1$. Therefore, the series in (3.1) diverges for all $x \in (0,\infty)$ and hence term-by-term integration is *not* permitted. This is not an unexpected result in view of the non-uniform convergence of the power series $\Sigma\, c_n s^n$, and consequently of the series $\Sigma\, \mathrm{e}^{-sx}c_n s^n$, in the s range $[0,\infty]$. These series converge uniformly only in the s interval $[0,R]$, $R<\infty$ (cf any textbook on classical analysis). The impossibility of expressing $g(x)$ as a series in $1/x$ for $x<\infty$ proves that the solutions can *not* be obtained by introducing $\xi=1/x$ in (2.13). This feature, in conjunction with the appearance of β in the denominators in (2.5) and (2.9), strongly suggests that these solutions may not be accessible to conventional perturbation theory.

The structure of (3.1) implies that it might be considered as an asymptotic expansion of $g(x)$ for $x \gg 1$. If this is correct, then the truncation of the series in (3.1) for some finite n immediately shows that $g(x) \to 0$ as $x \to \infty$. In fact, as the solutions (2.5) are mathematically valid for arbitrarily large x_2, we can consider the limit $x \to \infty$, i.e. $x_2 \to \infty$, and its implications. We are going to show in appendix 2 that

$$|y_1(x)| < M/x, \qquad x \gg 1, \qquad 0 < M < \infty. \tag{3.3}$$

Hence $y_1(x)$ remains physical for *all* $x \in (0, \infty)$, as $y_1(x) \to 0$ for $x \to \infty$. That $y_1(x) \to 0$ as $x \to \infty$ despite the fact that it corresponds to a continuous spectrum is not surprising in the face of a similar asymptotic behaviour of the wavefunction relevant to the continuous hydrogen spectrum (Morse and Feshbach 1953, Sommerfeld 1967). In this respect we wish to refer to a very recent paper (Fernández and Castro 1982) where the Hamiltonian

$$H = -\tfrac{1}{2}\,\mathrm{d}^2/\mathrm{d}x^2 + V_1(x), \qquad x \in [x_1, x_2] \tag{3.4}$$

has been studied, the boundary conditions at x_1, x_2 being arbitrary, with *finite* x_1, x_2. The proposed perturbative formalism is applied to the pure quartic oscillator

$$V_1(x) = \beta x^4, \tag{3.5}$$

bounded by infinite walls, and it is valid provided β is positive and small. Consequently, the solutions (2.5), which hold also for $\alpha = 0$, are not obtainable by means of the method of Fernández and Castro (1982), because that method, irrespective of the boundary conditions at x_1, x_2, requires finite x_1, x_2 while (2.5) retains its validity for $x_2 \to \infty$.

An interesting point to be raised here is that the presence of the exponent $\frac{2}{3}$ in (2.20) and, hence, also in (2.21) is actually what engenders the validity of the basic (2.26), as will become apparent from appendix 1. Indeed, if we consider (2.10) for $x \in (-\infty, \infty)$, we again arrive at (2.13) where now $x \in (-\infty, \infty)$. On solving (2.13) with $x \in (-\infty, \infty)$, we obtain as usual the solution $g(x)$ in the form

$$g(x) = \sum_{n=0}^{\infty} d_n x^n, \qquad d_0 \neq 0, \qquad -\infty < x < \infty. \tag{3.6}$$

Thus, the d_n fulfil a four-term recurrence formula from which we get an expression for d_{n+1}/d_n, $n \gg 1$, similar to (2.20) but with the power $\frac{1}{3}$ in place of $\frac{2}{3}$. In such a case no definite statement can be made for the behaviour of (2.11) as $x \to \infty$, even if we consider the $\beta < 0$ case. Omitting, however, $x = 0$ by means of a cut-off distance $x_1 > 0$ allows us to use (2.14) and formulate theorem 2.1.

In the following we shall examine to what extent our results can be related to the usual anharmonic oscillator. Namely, in the case of the potential defined by (1.1), one of the main results of Simon (1970) concerns the proof of the asymptotic nature in β of the perturbation series for the energy $E(\beta)$:

$$E(\beta) = E(0) + \sum_{n=1}^{\infty} a_n \beta^n \qquad (\beta = \text{complex}). \tag{3.7}$$

The main physically plausible assumption needed for that proof is that (Simon 1970)

$V(x)$ in (1.1) is bounded *below*. For $\beta<0$ this implies that one has to introduce a cut-off at some finite, albeit arbitrarily large, distances $x_1'<0$, $x_2>0$ where $x_2=|x_1'|$ can be taken without loss of generality (due to the symmetry of the potential). Further, one has to assume the discreteness of the spectrum of

$$H(\beta)=p^2+\alpha x^2+\beta x^4 \tag{3.8}$$

at the bottom. These requirements are satisfied by bounding $V(x)$ by infinite walls, thus also fulfilling, to any desired degree of accuracy, by choosing x_2 to be appropriately large, the eigenvalue condition, built in all the procedures treating (1.1), that the eigenfunction of $H(\beta)$ tends to zero as $|x|\to\infty$. That is precisely the situation depicted by (2.2) and (2.4) on the half axis $x>0$, where $|V_0'|$ can be made arbitrarily large without having to modify the E-spectrum obtained in theorem 2.1, since by virtue of (3.3), $y_1(x)\to 0$ for $x\to\infty$.

It should be noted that since $\beta<0$ the classical force $2\alpha x-4|\beta|x^3$ is capable of sending a particle to ∞ in only a finite amount of time (Simon 1970). Quantum mechanically, this is manifested in $H(\beta)$ being *not* self-adjoint unless we incorporate in the treatment the condition that the eigenfunction of $H(\beta)$ approaches zero for $|x|\to\infty$. The solutions in (2.5), which are effectively valid for all $x>0$ with $\lim_{x\to\infty}y_1(x)=0$, give in fact on the half axis $x>0$ an exact analytic example for such a case.

In the three-dimensional case we replace (1.1) by

$$V(r)=\alpha r^2+\beta r^4, \qquad 0\leqslant r<\infty. \tag{3.9}$$

As all the properties of equation (1.1) can be extended to three dimensions (Simon 1970), which may correspond to more realistic models, the preceding discussion on the relation of our results to the standard anharmonic oscillator can be without any change applied to the s-waves case in three dimensions (Znojil 1981); we have only to replace x in all the relevant equations of § 2 with the variable $r\geqslant 0$. Now, since $V(r)$ goes smoothly to zero as $r\to 0$ the underlying physical situation should not change appreciably if we introduce a small cut-off distance r_1 and consider $V(r)=0$ for $0\leqslant r\leqslant r_1$. Hence, for $\beta<0$ and s-waves the solution for the continuous spectrum of such a model is simply $y_1(r)/r$, $0<r_1\leqslant r\leqslant r_2<\infty$, $y_1(r)$ being given by (2.5). Consequently we may argue that $y_1(r)/r$ could be a reasonable approximation to the exact solution for (3.9) in the case of the continuous spectrum pertaining to it, as $y_1(r)/r$ is essentially valid for *any* $r>0$.

Finally, as there is evidence (Bender and Wu 1969) that the analytic properties of the spectrum of (1.1) are probably present in more realistic field theories than the zero-space-dimensional field theory corresponding to (1.1), it may be worthwhile to try to investigate the potential in (2.2)–(2.4) for general complex β-values with the aim of gaining some idea of the apparent complexity of such theories.

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Appendix 1.

In this appendix, we use complex analysis to investigate the basic sum in (2.25). Consider the function

$$f(z)=\frac{1}{\Gamma(n+1-z)[\Gamma(2z+1)]^{2/3}}, \qquad z=x+\mathrm{i}y \qquad (\Gamma(Z)=\text{Gamma function}). \tag{A1.1}$$

Then S_n can be written, by applying the method for the conversion of a sum into an integral (Morse and Feshbach 1953),

$$S_n=\frac{1}{2\mathrm{i}}\oint \Gamma(n+1)f(z)\,\mathrm{cosec}(\pi z)\,\mathrm{d}z. \tag{A1.2}$$

The contour integral in (A1.2) is taken counterclockwise around a closed rectangular contour encircling the points $0, 1, 2, 3, \ldots, n$. Thus it breaks up into four integrals, the first of which is (omitting $1/2\mathrm{i}$)

$$I_1=2\Gamma(n+1)\int_{-L}^{L}\frac{\mathrm{e}^{\mathrm{i}\pi/4}}{\Gamma(n+1+\frac{1}{4}-\mathrm{i}y)[\Gamma(-\frac{2}{4}+1+2\mathrm{i}y)]^{2/3}(\mathrm{e}^{-\pi y}-\mathrm{i}\,\mathrm{e}^{\pi y})}\,\mathrm{d}y \tag{A1.3}$$

with $z=-\frac{1}{4}+\mathrm{i}y$. On using the relation (Abramowitz and Stegun 1956)

$$|\Gamma(\tfrac{1}{2}+2\mathrm{i}y)|=\pi^{1/2}/(\cosh 2\pi y)^{1/2}, \tag{A1.4}$$

and since (Abramowitz and Stegun 1956) $|\Gamma(\bar{Z})|=|\Gamma(Z)|$, we obtain for I_1 in (A1.3) after a few elementary steps

$$|I_1|\leqslant\frac{4}{(2\pi)^{1/3}}\Gamma(n+1)\int_0^L\frac{\mathrm{e}^{\pi y}(\mathrm{e}^{2\pi y}+\mathrm{e}^{-2\pi y})^{1/3}}{|\Gamma(n+1+\frac{1}{4}+\mathrm{i}y)||1-\mathrm{i}\,\mathrm{e}^{2\pi y}|}\,\mathrm{d}y. \tag{A1.5}$$

For finite L and $n\gg1$ it can be easily seen by applying the asymptotic formula for the Gamma function that the right-hand side of equation (A1.5) can be made arbitrarily small for sufficiently large n. In view, however, of the considerations concerning the integrals along the other sides of the rectangular contour, we must have in (A1.5) $L\gg1$. Thus we shall take the following formula (Morse and Feshbach 1953) valid for $|Z|\gg1$ with $Z=X+\mathrm{i}Y$:

$$|\Gamma(X+1+\mathrm{i}Y)|=(2\pi)^{1/2}(X^2+Y^2)^{(2X+1)/4}\,\mathrm{e}^{-(Y\phi+X)}, \qquad \phi=\tan^{-1}(Y/X). \tag{A1.6}$$

Now for $n\gg1$ we get by equation (A1.6)

$$\frac{\Gamma(n+1)}{|\Gamma(n+1+\frac{1}{4}+\mathrm{i}y)|}=\frac{\mathrm{e}^{\phi y}}{n^{1/4}[1+y^2/(n+\frac{1}{4})^2]^{n/2+3/8}}, \qquad \phi=\tan^{-1}\frac{y}{n+\frac{1}{4}}. \tag{A1.7}$$

Further, we let L, for given n, be defined by

$$L=n+\tfrac{1}{4}. \tag{A1.8}$$

Then, by (A1.7), ϕ varies between 0 and $\pi/4$. Hence equation (A1.5) becomes for $n\gg1$ by virtue of (A1.7) and (A1.8)

$$|I_1|\leqslant\frac{4}{(2\pi)^{1/3}n^{1/4}}\int_0^L\frac{\mathrm{e}^{y5\pi/4}(\mathrm{e}^{2\pi y}+\mathrm{e}^{-2\pi y})^{1/3}}{(1+\mathrm{e}^{4\pi y})^{1/2}}\,\mathrm{d}y<\frac{4}{(2\pi)^{1/3}n^{1/4}}\int_0^\infty\frac{\cdots}{\cdots} \tag{A1.9}$$

where, in writing down the first integral in (A1.9), we have taken account of the fact that

$$\{[y/(n+\tfrac{1}{4})]^2+1\}^{n/2+3/8}\geqslant 1 \tag{A1.9a}$$

and that the maximum value of ϕ is $\pi/4$. Consequently

$$|I_1|<4(2\pi)^{-1/3}Mn^{-1/4} \qquad (n\gg 1, L\gg 1, L=n+\tfrac{1}{4}), \tag{A1.10}$$

M being the finite value of the last integral in (A1.9), which clearly exists, as the integrand is finite for $y\geqslant 0$ and goes to 0 for $y\to\infty$.

For the second integral along the contour in (A1.2) we obtain with $z=x-\mathrm{i}L$

$$|I_2|\leqslant 2\Gamma(n+1)\int_{-1/4}^{n+1/4}\frac{\mathrm{e}^{\pi L}}{|\Gamma(n-x+1+\mathrm{i}L)||\Gamma(2x+1+2\mathrm{i}L)|^{2/3}|\mathrm{e}^{2\pi(\mathrm{i}x+L)}-1|}\,\mathrm{d}x. \tag{A1.11}$$

Since $L\gg 1$ we can replace the Gamma functions in (A1.11) by (A1.6), which is applicable as long as $(X^2+Y^2)^{1/2}\gg 1$, a condition satisfied here. Bearing in mind that also $n\gg 1$ and (A1.8), we deduce after some simple manipulations

$$|I_2|\leqslant\frac{2C}{(2\pi)^{1/3}\,\mathrm{e}^{1/4}}\int_{-1/4}^{n+1/4}\{\exp\{x/3-\ln(n)[(x+1)/3]+L(\phi+4\phi'/3-\pi)\}\}\,\mathrm{d}x, \tag{A1.12}$$

$$\phi=\tan^{-1}\frac{L}{n-x},\qquad \phi'=\tan^{-1}\frac{L}{x},\qquad C=\frac{1}{1-\mathrm{e}^{-2\pi L}},\qquad \frac{1}{\mathrm{e}^{2\pi L}-1}>\frac{1}{|\mathrm{e}^{2\pi(\mathrm{i}x+L)}-1|}. \tag{A1.13}$$

In the integrand of (A1.12) we have omitted the terms

$$\left[\left(\frac{n-x}{L}\right)^2+1\right]^{-(2n-2x+1)/4},\qquad \left[\left(\frac{x}{L}\right)^2+1\right]^{-(4x+1)/6},\qquad 2^{-(4x+1)/3} \tag{A1.14}$$

as they are always $\leqslant 1$. As, further, a simple calculation shows, the maximum value of $\phi+(4\phi'/3)-\pi$ is $\cong -\pi/12$. Then performing the remaining integral in (A1.12) we deduce

$$|I_2|\leqslant\frac{6C\,\mathrm{e}^{-\pi/48}}{(2\pi)^{1/3}\,\mathrm{e}^{1/4}\,\mathrm{e}^{\pi n/12}}\left[\frac{\mathrm{e}^{-1/12}}{n^{1/4}[\ln(n)-1]}-\frac{1}{n^{1/3}[\ln(n)-1]}\left(\frac{\mathrm{e}}{n}\right)^{(4n+1)/12}\right]$$
$$(n\gg 1, L\gg 1, L=n+\tfrac{1}{4}). \tag{A1.15}$$

The next integral on the contour in equation (A1.2) is easily seen to fulfil with $z=n+\frac{1}{4}+\mathrm{i}y$, $L=n+\frac{1}{4}$,

$$|I_3|\leqslant 4\Gamma(n+1)\int_0^L\frac{1}{|\Gamma(\frac{3}{4}+\mathrm{i}y)||\Gamma(2n+\frac{1}{2}+1+2\mathrm{i}y)|^{2/3}|\mathrm{e}^{-\pi y}+\mathrm{i}\mathrm{e}^{\pi y}|}\,\mathrm{d}y. \tag{A1.16}$$

As $n\gg 1$ we can utilise (A1.6) for the Gamma functions in (A1.16). Thus

$$|I_3|\leqslant\left(\frac{\mathrm{e}}{n}\right)^{n/3}\frac{(2\pi)^{1/6}}{n^{1/6}2^{(4n+2)/3}}\int_0^L\frac{\exp\{4y[\tan^{-1}y/(n+\frac{1}{4})]/3\}}{|\Gamma(\frac{3}{4}+\mathrm{i}y)||\mathrm{e}^{-\pi y}+\mathrm{i}\,\mathrm{e}^{\pi y}|}\,\mathrm{d}y. \tag{A1.17}$$

In the integrand of (A1.17) we have discarded the term

$$\{[y/(n+\tfrac{1}{4})]^2+1\}^{-(2n+1)/3}\leqslant 1. \tag{A1.18}$$

Now, the integral, I, on the right-hand side of (A1.17) satisfies

$$I \leqslant \int_0^L \frac{e^{\pi y/3}}{|\Gamma(\frac{3}{4}+iy)||e^{-\pi y}+i\,e^{\pi y}|}\,dy < M' \qquad \left(\frac{\pi}{4}=\max\left(\tan^{-1}\frac{y}{n+\frac{1}{4}}\right)\right) \tag{A1.19}$$

where

$$M'=\int_0^\infty \frac{e^{\pi y/3}}{|\Gamma(\frac{3}{4}+iy)||e^{-\pi y}+i\,e^{\pi y}|}\,dy. \tag{A1.19a}$$

M' exists, as the application of (A1.6) to $|\Gamma(\frac{3}{4}+iy)|$ for $y \gg 1$ shows. (The relevant integrand is finite for $y \geqslant 0$ and tends to 0 as $y \to \infty$.) Hence,

$$|I_3| < \left(\frac{e}{n}\right)^{n/3} \frac{(2\pi)^{1/6}}{n^{1/6}2^{(4n+2)/3}} M' \qquad (n \gg 1, L \gg 1, L = n+\tfrac{1}{4}). \tag{A1.20}$$

The fourth and final integral, I_4, where $z = x + iL$ and x varies from $n+\frac{1}{4}$ to $-\frac{1}{4}$, is easily shown to satisfy (A1.11) and, therefore, also (A1.15). On combining further (A1.10), (A1.15) and (A1.20), we observe that $|S_n|$ in (A1.2) from a certain large but *finite* n, say n_1, onwards cannot exceed a finite bound. As a consequence we can find a finite $N > n_1$ such that

$$|S_n| < n, \; n \geqslant N. \tag{A1.21}$$

This N is essentially determined from $|I_1| < N$ since I_2, I_3 and I_4 fall much more rapidly. If we consider (A1.21) in place of (2.26), then we will obtain that $|\Sigma_1'|$ cannot behave stronger than $e^z(1+z)$ + polynomial of degree N in z. This clearly does not affect the existence of the integral in (2.14). A characteristic feature, however, of (A1.6), on which actually (A1.21) is based, is that it is valid also for moderately large X or Y. In fact the accuracy of (A1.6) is surprising even for small (Jeffreys and Jeffreys 1956) $|Z|$, i.e. $|Z| = 1, 2, \ldots$. Thus (A1.21) most probably holds for small n too.

We have carried out a numerical investigation of the sum S_n and have followed its behaviour up to $n = 500$. The structure of S_n indicates that even for small n, for instance $n = 20$, a large number of manipulations are performed in which huge numbers alternating in sign are added. This causes round-off errors and despite the fact that the calculation was performed to 32 decimal places (quadruple-precision mode), the capacity of the computer to manipulate these numbers is rapidly exceeded after $n = 440$. For $n = 450$ we have terms of the order 10^{27} which alternate in sign. Double precision can get us only to about $n = 135$.

In table 1 we present some of the results of the numerical calculation. It is interesting to note that (cf figure 1(a), (b)):

(i) S_n is negative for $n \geqslant 2$.

(ii) $|S_n| < 1$ for $n \geqslant 1$. Also S_n has an absolute minimum for $n = 5$, a relative maximum at $n = 22$ and a relative minimum for $n = 34$. For $n > 34$, $|S_n|$ decreases monotonically and tends to 0 as $n \to \infty$, albeit slowly. This is obviously predicted by (A1.10), (A1.15) and (A1.20). It is perhaps worth pointing out that the slow rate at which $|S_n| \to 0$ for $n \to \infty$ is implied by (A1.10). (Note the factor $n^{1/4}$ in the denominator.)

Taking account of (i)–(ii) we can write down (2.26).

Finally, we wish to remark that the presence of the fractional exponent $\frac{2}{3}$ is what actually ensures the validity of (A1.15) and (A1.20). Had we $\frac{1}{3}$ instead, it would have been no longer possible to prove that $|I_2|$, $|I_3|$ and $|I_4|$ are bounded by relations similar

Table 1. S_n as a function of n.

n	S_n	n	S_n	n	S_n	n	S_n
0	1.000 000	24	−0.017 330	48	−0.018 748	80	−0.011 897
1	0.370 039	25	−0.018 352	49	−0.018 339	90	−0.010 790
2	−0.019 546	26	−0.019 479	50	−0.017 951	100	−0.009 886
3	−0.243 447	27	−0.020 593	51	−0.017 585	110	−0.009 138
4	−0.355 942	28	−0.021 615	52	−0.017 239	120	−0.008 508
5	−0.395 981	29	−0.022 496	53	−0.016 912	130	−0.007 969
6	−0.391 090	30	−0.023 208	54	−0.016 605	140	−0.007 501
7	−0.360 357	31	−0.023 741	55	−0.016 314	150	−0.007 092
8	−0.316 701	32	−0.024 098	56	−0.016 040	160	−0.006 730
9	−0.268 587	33	−0.024 289	57	−0.015 780	170	−0.006 408
10	−0.221 309	34	−0.024 331	58	−0.015 534	180	−0.006 120
11	−0.177 942	35	−0.024 242	59	−0.015 300	190	−0.005 859
12	−0.140 051	36	−0.024 043	60	−0.015 077	200	−0.005 623
13	−0.108 195	37	−0.023 753	61	−0.014 865	210	−0.005 407
14	−0.082 299	38	−0.023 393	62	−0.014 661	220	−0.005 210
15	−0.061 909	39	−0.022 978	63	−0.014 466	230	−0.005 028
16	−0.046 375	40	−0.022 525	64	−0.014 277	240	−0.004 861
17	−0.034 965	41	−0.022 048	65	−0.014 096	250	−0.004 706
18	−0.026 951	42	−0.021 557	66	−0.013 921	260	−0.004 561
19	−0.021 647	43	−0.021 063	67	−0.013 751	270	−0.004 427
20	−0.018 442	44	−0.020 573	68	−0.013 586	280	−0.004 301
21	−0.016 809	45	−0.020 092	69	−0.013 426	290	−0.004 184
22	−0.016 306	46	−0.019 626	70	−0.013 270	300	−0.004 074
23	−0.016 575	47	−0.019 177	71	−0.013 118		

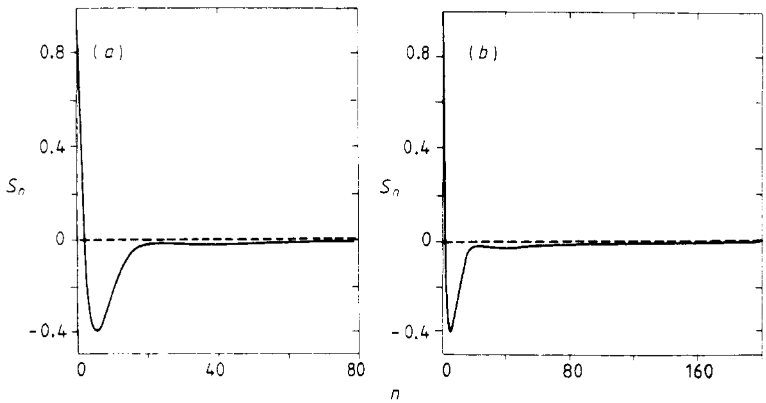

Figure 1. S_n as a function of n.

to (A1.15) and (A1.20), although the condition equivalent to (A1.10) would still be valid. Indeed, we have replaced $\frac{2}{3}$ by $\frac{1}{3}$ in S_n and observed that the computer program yields, even for small n, large values in sharp contrast to the results pertaining to $\frac{2}{3}$. It should also be noted that (A1.21) cannot be obtained by manipulating known sums and comparing them with S_n by application of the Abel inequality, which is central to the theory of series, simply because the terms in S_n depend on n *themselves* and all known procedures become inapplicable.

Appendix 2.

The function $g(x)$ in (2.14) can be written as

$$g(x)=\int_0^R e^{-sx}f(s)\,ds+\int_R^\infty e^{-sx}f(s)\,ds. \tag{A2.1}$$

On denoting the maximum value of $|f(s)|$ for $s\in[0,R]$ by M_R and observing that, since $f(s)$ is given by a convergent series in the range $[0,\infty)$, $M_R<\infty$, we obtain for the first integral, J_1, in (A2.1)

$$|J_1|\leqslant M_R\int_0^R e^{-sx}\,ds=M_R\frac{1}{x}(1-e^{-Rx}). \tag{A2.2}$$

We choose now a sufficiently large but *finite* R and denote by $f_{as}(s)$ the asymptotic approximation of $f(s)$. Then we have for the remainder, $r(s)$, the exact relation $r(s)=f(s)-f_{as}(s)$, $s\gg1$. Owing to $|r(s)|<\varepsilon$, $\varepsilon>0$, for $s>R\gg1$, and to (2.30), we deduce for (A2.1) by using (A2.2)

$$|g(x)|\leqslant\frac{M_R}{x}(1-e^{-Rx})+\int_R^\infty e^{-sx}(1+Ls+L^2s^2)\,ds+\frac{1}{L}\int_R^\infty\frac{e^{-sx}}{s}\,ds+\varepsilon\int_R^\infty e^{-sx}\,ds. \tag{A2.3}$$

On recalling the definition of the exponential integral, $E_1(x)$, we get

$$E_1(x)=\int_1^\infty\frac{e^{-sx}}{s}\,ds\geqslant\int_R^\infty\frac{e^{-sx}}{s}\,ds \tag{A2.4}$$

and, therefore, (A2.3) yields

$$|g(x)|\leqslant\frac{M_R}{x}(1-e^{-Rx})+e^{-Rx}\left(\frac{1+\varepsilon+LR+L^2R^2}{x}+\frac{L+2RL^2}{x^2}+\frac{2L^2}{x^3}\right)+\frac{1}{L}E_1(x). \tag{A2.5}$$

Letting $x\to\infty$, we observe from (A2.5) that $g(x)\to0$ as $x\to\infty$ and that $g(x)$ for $x\gg1$ falls at least as rapidly as $1/x$, due to the presence of the factor e^{-Rx} and the asymptotic behaviour of $E_1(x)$

$$E_1(x)=e^{-x}/x,\qquad x\gg1. \tag{A2.6}$$

The proof of $g(x)\to0$ for $x\to\infty$ can be done simply by looking at the integrand in (2.14). The above procedure, however, gives also the rate at which $g(x)\to0$ as $x\to\infty$. Moreover, it reveals that (3.1), although giving the correct result $g(x)\to0$ for $x\to\infty$, cannot be considered as the asymptotic series for $g(x)$, not least because of the absence of the (in the Poincaré sense) necessary remainder.

By virtue now of (2.5) the truth of (3.3) becomes obvious.

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