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# Energy bounds for a class of singular potentials and some related series

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**Abstract**
Perturbation expansions up to third order for the generalized spiked harmonic oscillator Hamiltonians $H = -\frac{d^2}{dx^2} + x^2 + \frac{A}{x^2} + \frac{\lambda}{x^\alpha}\big(A \geqslant 0, 2\gamma > \alpha, \gamma = 1 + \frac{1}{2}\sqrt{1+4A}\big)$ and small values of the coupling $\lambda > 0$, are developed. Upper and lower bounds for the eigenvalues are computed by the procedure of Burrows *et al* (1987 *J. Phys. A: Math. Gen.* **20** 889–97) for assessing the accuracy of a truncated perturbation expansion. Closed-form sums for some related perturbation double infinite series then immediately follow as a result of this investigation.

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## 1. Introduction

It is well known that, although many perturbation expansions diverge, they may actually be asymptotic expansions whose first few terms can yield good approximations. The family of spiked harmonic oscillator Hamiltonians

$$H = H_0 + \lambda V = -\frac{d^2}{dx^2} + x^2 + \frac{\lambda}{x^\alpha} \qquad (0 \leqslant x < \infty) \tag{1.1}$$

affords interesting examples of this phenomenon. Harrell [1] has shown that the familiar Rayleigh–Schrödinger perturbation series diverge accordingly as $n \geqslant \frac{1}{\alpha-2}$, where $n$ is the order of the Rayleigh–Schrödinger term. For example, the first-order perturbation correction diverges for $\alpha \geqslant 3$, while the second-order correction term diverges if $\alpha \geqslant \frac{5}{2}$, and so on. In a series of articles, Aguilera-Navarro *et al* [2], Estvéz-Bretón *et al* [3] and Znojil [4] have shown for the case of $\alpha < 5/2$, the so-called non-singular case, that the perturbation series of the ground-state energy up to the second-order corrections is given by

$$E(\lambda,\alpha) = 3 + \frac{\Gamma\left(\frac{3-\alpha}{2}\right)}{\Gamma\left(\frac{3}{2}\right)}\lambda - \frac{\Gamma^2\left(\frac{3-\alpha}{2}\right)}{\Gamma^2\left(\frac{3}{2}\right)}\sum_{i=1}^{\infty}\frac{\left(\frac{\alpha}{2}\right)_i^2}{4i\left(\frac{3}{2}\right)_i i!}\lambda^2 + \cdots \qquad \text{for} \quad \alpha < 5/2. \tag{1.2}$$

Based on resummation techniques, an analysis of Aguilera-Navarro *et al* [2] showed that

$$\sum_{i=1}^{\infty}\frac{\left(\frac{\alpha}{2}\right)_i^2}{4i\left(\frac{3}{2}\right)_i i!}=\sum_{i=1}^{\infty}\frac{\left(\frac{\alpha}{2}\right)_i^2}{4(i+1)\left(\frac{3}{2}\right)_i i!}+\sum_{i=1}^{\infty}\frac{\left(\frac{\alpha}{2}\right)_i^2}{4i(i+1)\left(\frac{3}{2}\right)_i i!}$$
$$=\frac{1}{8\left(\frac{\alpha}{2}-1\right)^2}\left[{}_2F_1\left(\frac{\alpha}{2}-1,\frac{\alpha}{2}-1;\frac{1}{2};1\right)-1-2\left(\frac{\alpha}{2}-1\right)^2\right]$$
$$+\sum_{i=1}^{\infty}\frac{\left(\frac{\alpha}{2}\right)_i^2}{4i(i+1)\left(\frac{3}{2}\right)_i i!} \tag{1.3}$$

where ${}_2F_1(a,b;c;z)$ is the known Gauss hypergeometric function [5] with circle of convergence $|z|=1$. For the limiting case $\alpha\to 2$, the first term on the right-hand side of (1.3) was shown by Estv́ez-Bretón *et al* [3] using l'Hôpital's rule to be

$$\lim_{\alpha\to 2}\frac{1}{8\left(\frac{\alpha}{2}-1\right)^2}\left[{}_2F_1\left(\frac{\alpha}{2}-1,\frac{\alpha}{2}-1;\frac{1}{2};1\right)-1-2\left(\frac{\alpha}{2}-1\right)^2\right]=\frac{\pi^2}{16}-\frac{1}{4}. \tag{1.4}$$

Znojil, soon afterwards [4], showed elegantly that (1.4) follows immediately by manipulating the Maclaurin expansion of the gamma function. Recently, Hall and Saad [6–10] investigated a larger class, the so-called generalized spiked harmonic oscillator Hamiltonians

$$H=H_0+\lambda V=-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+x^2+\frac{A}{x^2}+\frac{\lambda}{x^\alpha}\qquad (A\geqslant 0). \tag{1.5}$$

The Gol'dman and Krivchenkov Hamiltonian $H_0=-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+x^2+\frac{A}{x^2}$, which admits the exact solutions

$$\psi_n(x)=(-1)^n\sqrt{\frac{2(\gamma)_n}{n!\Gamma(\gamma)}}x^{\gamma-\frac{1}{2}}\,\mathrm{e}^{-\frac{1}{2}x^2}\,{}_1F_1(-n,\gamma,x^2) \tag{1.6}$$

with exact eigenenergies

$$E_n=4n+2\gamma\qquad n=0,1,2,\ldots\qquad \gamma=1+\tfrac{1}{2}\sqrt{1+4A} \tag{1.7}$$

is regarded as the unperturbed part, and the operator $V(x)=x^{-\alpha}$ as the perturbed part. They obtained [8] the energy expansion up to the second order as

$$E(\lambda,\alpha)=2\gamma+\frac{\Gamma\left(\gamma-\frac{\alpha}{2}\right)}{\Gamma(\gamma)}\lambda-\lambda^2\frac{\alpha^2}{16\gamma}\frac{\Gamma^2\left(\gamma-\frac{\alpha}{2}\right)}{\Gamma^2(\gamma)}$$
$$\times\,{}_4F_3\left(1,1,1+\frac{\alpha}{2},1+\frac{\alpha}{2};2,2,\gamma+1;1\right)+\cdots \tag{1.8}$$

valid for $\alpha<\gamma+1$, where $\gamma=1+\frac{1}{2}\sqrt{1+4A}$. A closed-form sum for the infinite series in (1.2) appears as a special case. In particular, for $\gamma=3/2$ or $A=0$, equation (1.8), for $\alpha<\frac{5}{2}$, reduces to

$$E(\lambda,\alpha)=3+\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3-\alpha}{2}\right)\lambda-\lambda^2\frac{\alpha^2}{48}\frac{\Gamma^2\left(\frac{3-\alpha}{2}\right)}{\Gamma^2(\gamma)}{}_4F_3\left(1,1,1+\frac{\alpha}{2},1+\frac{\alpha}{2};2,2,\frac{5}{2};1\right)+\cdots$$

and closed-form sums of the infinite series in (1.2) follow immediately. Furthermore, for $\alpha=2$, since

$${}_4F_3(1,1,2,2;2,2,\gamma+1;1)={}_2F_1(1,1;\gamma+1;1)=\frac{\Gamma(\gamma+1)\Gamma(\gamma-1)}{\Gamma(\gamma)\Gamma(\gamma)}=\frac{\gamma}{(\gamma-1)}$$

by means of Chu–Vandermonde theorem [5]

$${}_2F_1(a,b;c;1)=\frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}\qquad\text{for}\quad c-a-b>0 \tag{1.9}$$

the perturbation expansion (1.8) takes the very simple form

$$E(\lambda, \alpha = 2) = 2\gamma + \frac{\lambda}{(\gamma - 1)} - \frac{\lambda^2}{4(\gamma - 1)^3} + \cdots. \tag{1.10}$$

This is obtained, as expected, by means of Taylor's expansion of the exact energy $2 + \sqrt{1 + 4(A + \lambda)}$ about $\lambda = 0$. In order to understand the result (1.4), however, we should note first

$$\begin{aligned}\sum_{i=1}^{\infty} \frac{\left(\frac{\alpha}{2}\right)_i^2}{4(i+1)(\gamma)_i i!} &= \frac{(\gamma - 1)}{4\left(\frac{\alpha}{2} - 1\right)^2} \left[ {}_2F_1\left(\frac{\alpha}{2} - 1, \frac{\alpha}{2} - 1; \gamma - 1; 1\right) - 1 - \frac{\left(\frac{\alpha}{2} - 1\right)^2}{(\gamma - 1)} \right] \\ &= \frac{(\gamma - 1)}{4\left(\frac{\alpha}{2} - 1\right)^2} \left[ \frac{\Gamma(\gamma - 1)\Gamma(\gamma - \alpha + 1)}{\Gamma\left(\gamma - \frac{\alpha}{2}\right)\Gamma\left(\gamma - \frac{\alpha}{2}\right)} - 1 - \frac{\left(\frac{\alpha}{2} - 1\right)^2}{(\gamma - 1)} \right] \\ &= \frac{(\gamma - 1)}{4\left(\frac{\alpha}{2} - 1\right)^2} \left[ \frac{\Gamma(\gamma - 1)\Gamma(\gamma - \alpha + 1)}{\Gamma(\gamma - \frac{\alpha}{2})\Gamma\left(\gamma - \frac{\alpha}{2}\right)} - 1 \right] - \frac{1}{4}\end{aligned}$$

where we have used (1.9). Now since

$$\lim_{\alpha \to 2} \frac{1}{\left(\frac{\alpha}{2} - 1\right)^2} \left[ \frac{\Gamma(\gamma - 1)\Gamma(\gamma - \alpha + 1)}{\Gamma\left(\gamma - \frac{\alpha}{2}\right)\Gamma\left(\gamma - \frac{\alpha}{2}\right)} - 1 \right] = \psi^{(1)}(\gamma - 1)$$

we have

$$\sum_{i=1}^{\infty} \frac{(1)_i^2}{(i+1)(\gamma)_i i!} = \frac{1}{2\gamma} {}_3F_2(1, 2, 2; 3, \gamma + 1; 1) = (\gamma - 1)\psi^{(1)}(\gamma - 1) - 1 \qquad \text{for} \quad \gamma > 1 \tag{1.11}$$

where $\psi^{(1)}(z)$ is the first derivative of the digamma function (or logarithmic derivative of the gamma function [11]) . Further, since $\psi^{(1)}\left(\frac{1}{2}\right) = \frac{\pi^2}{2}$, the result of (1.4) follows immediately by replacing $\gamma$ with 3/2 in (1.11).

The interesting feature of expression (1.8) is that, it can be applied to the ground-state eigenenergy at the bottom of each angular momentum subspace labelled by $l = 0, 1, 2, \ldots,$ in $N$ dimensions: we just need to replace $A$ with $A \to A + \left(l + \frac{1}{2}(N - 1)\right)\left(l + \frac{1}{2}(N - 3)\right)$. Furthermore, as we shall prove in the next section, for $\alpha = 4$ and $\gamma > 3$ (or $A > 3.75$), the perturbation expansion (1.8) takes the very simple form

$$E(\lambda, \alpha = 4) = 2\gamma + \frac{\lambda}{(\gamma - 1)(\gamma - 2)} - \lambda^2 \frac{4\gamma^2 - 15\gamma + 13}{4(\gamma - 1)^3(\gamma - 2)^3(\gamma - 3)} + \cdots \tag{1.12}$$

where $\psi$ is the digamma function. For $\alpha = 6$ and $\gamma > 5$ (or $A > 15.75$), (1.8) becomes

$$\begin{aligned}E(\lambda, \alpha = 6) = 2\gamma &+ \frac{\lambda}{(\gamma - 1)(\gamma - 2)(\gamma - 3)} - \frac{\Gamma^2(\gamma - 3)}{8\Gamma^2(\gamma)} \left( \frac{(\gamma - 2)(\gamma - 1)}{(\gamma - 5)(\gamma - 4)} \right. \\ &\left. + \frac{2(\gamma - 1)}{(\gamma - 4)} + \frac{40 - 57\gamma + 8\gamma^2 - \gamma^3}{(\gamma - 3)(\gamma - 2)(\gamma - 1)} \right) \lambda^2 + \cdots.\end{aligned} \tag{1.13}$$

In section 2 we shall extend these perturbation expansions to third-order corrections. In section 3, we shall discuss upper and lower bounds for the eigenvalues by the procedure of Burrows *et al* [12] for assessing the accuracy of a truncated perturbation expansion. These bounds will shed some light on the question regarding the acceleration of the variational method. Our conclusions and some remarks concerning the sums of some double infinite series will be given in section 4.

The functions ${}_1F_1$ and ${}_4F_3$, mentioned above, are special cases of the generalized hypergeometric function [13]

$$ {}_pF_q(\alpha_1, \alpha_2, \ldots, \alpha_p; \beta_1, \beta_2, \ldots, \beta_q; z) = \sum_{k=0}^{\infty} \frac{\prod_{i=1}^{p}(\alpha_i)_k}{\prod_{j=1}^{q}(\beta_j)_k} \frac{z^k}{k!} \tag{1.14} $$

where $p$ and $q$ are non-negative integers, and none of the $\beta_j$ $(j = 1, 2, \ldots, q)$ is equal to zero or to a negative integer. If the series does not terminate (that is to say, none of the $\alpha_i$, $i = 1, 2, \ldots, p$, is a negative integer), then the series, in the case $p = q + 1$, converges or diverges accordingly as $|z| < 1$ or $|z| > 1$. For $z = 1$, the series is convergent provided $\sum_{j=1}^{q} \beta_j - \sum_{i=1}^{p} \alpha_i > 0$. Here $(a)_n$, the shifted factorial (or *Pochhammer symbol*), is defined by

$$ (a)_0 = 1 \qquad (a)_n = a(a+1)(a+2)\cdots(a+n-1) = \frac{\Gamma(a+n)}{\Gamma(a)} \qquad n = 1, 2, \ldots. \tag{1.15} $$

## 2. Third-order perturbation expansions

In this section, we will expand the perturbation expansions (1.8) to the third-order correction. Although, we will concentrate on the cases of $\alpha = 4$ and $\alpha = 6$, since they are the most relevant in the literature [15–24], for other values of $\alpha$ the procedure is similar. In order to lay the foundation of the perturbation expansion (1.8), we first review the Rayleigh–Schrödinger perturbation theory for a non-degenerate case [25]. The fundamental problem in perturbation theory is the solution of the Schrödinger equation $H\phi = E(\lambda)\phi$ when $H = H_0 + \lambda V$. The basic assumption is that $\phi$ and $E(\lambda)$ may be expanded in power series in the perturbation parameter $\lambda$:

$$ \phi = \psi_0 + \sum_{i=1}^{\infty} \lambda^i \phi_i \qquad E(\lambda) = E_0 + \sum_{i=1}^{\infty} \lambda^i \epsilon_i. \tag{2.1} $$

Here $\psi_0$ is a solution to the unperturbed problem $H_0\psi_0 = E_0\psi_0$. We also choose the normalization $(\psi_0, \phi) = 1$, which implies that the higher-order corrections $\phi_1, \phi_2, \ldots,$ are orthogonal to $\psi_0$. Perturbation theory tells us in this case that

$$ \epsilon_1 = (\psi_0, V\psi_0) \quad \epsilon_2 = (\psi_0, V\phi_1) \quad \epsilon_3 = (\phi_1, V\phi_1) - \epsilon_1(\phi_1, \phi_1) \quad \ldots \tag{2.2} $$

or, equivalently [26],

$$ \begin{aligned} &\epsilon_1 = (\psi_0, V\psi_0) \quad \epsilon_2 = \sum_{i=1}^{\infty} \frac{|V_{0i}|^2}{E_i - E_0} \\ &\epsilon_3 = \sum_{s=1}^{\infty}\sum_{k=1}^{\infty} \frac{V_{0s}V_{sk}V_{k0}}{(E_s - E_0)(E_k - E_0)} - \epsilon_1 \sum_{i=1}^{\infty} \frac{|V_{0i}|^2}{(E_i - E_0)^2} \quad \ldots. \end{aligned} \tag{2.3} $$

From (2.2) it is clear that the first-order wavefunction $\phi_1$ determines the energy to the third order. The matrix elements $V_{ij} = (\psi_i, V\psi_j)$ in (2.3) are computed by means of the basis solution $\{\psi_n\}$ of the unperturbed Hamiltonian $H_0$. For the generalized spiked harmonic oscillator Hamiltonian (1.5), the expectation values of the operator $V(x) = x^{-\alpha}$ with respect to the Gol'dman and Krivchenkov basis (1.6) are given explicitly by

$$ V_{ij} = (-1)^{i+j} \frac{\left(\frac{\alpha}{2}\right)_i \Gamma\left(\gamma - \frac{\alpha}{2}\right)}{(\gamma)_i \Gamma(\gamma)} \sqrt{\frac{(\gamma)_i(\gamma)_j}{i!j!}}\, {}_3F_2\left(-j, \gamma - \frac{\alpha}{2}, 1 - \frac{\alpha}{2}; \gamma, 1 - i - \frac{\alpha}{2}; 1\right). \tag{2.4} $$

Of particular interest is

$$V_{i0} = V_{0i} = (-1)^i \frac{\left(\frac{\alpha}{2}\right)_i}{(\gamma)_i} \sqrt{\frac{(\gamma)_i}{i!}} \frac{\Gamma\left(\gamma - \frac{\alpha}{2}\right)}{\Gamma(\gamma)}. \tag{2.5}$$

Recently, Hall *et al* [27, 28] have shown that the first-order correction of the wavefunction, in the case of $\alpha = 2$, is given by

$$\phi_1(x) = \frac{1}{\sqrt{2}} \frac{x^{\gamma-\frac{1}{2}} \,\mathrm{e}^{-\frac{x^2}{2}}}{(\gamma-1)\sqrt{\Gamma(\gamma)}} \left[\log(x) - \frac{1}{2}\psi(\gamma)\right] \qquad \text{for} \quad \gamma > 1. \tag{2.6}$$

Therefore from (2.2) and (2.3), by using (2.5), we have

$$-\frac{\Gamma^2(\gamma-1)}{\Gamma^2(\gamma)} \sum_{i=1}^{\infty} \frac{(1)_i^2}{4i(\gamma)_i i!} = \int_0^\infty x^{-2}\psi_0(x)\phi_1(x)\,\mathrm{d}x = -\frac{1}{4(\gamma-1)^3}$$

as shown previously using the summation technique. This idea can be used to obtain a simple form by expressing ${}_4F_3$ in (1.8) in terms of elementary functions. These indeed are facilitated by the closed expression of the first-order correction of the wavefunctions developed earlier [27, 28]. In the case $\alpha = 4$, the first-order correction of the wavefunction reads

$$\phi_1(x) = \frac{1}{2\sqrt{2}} \frac{x^{\gamma-\frac{1}{2}} \,\mathrm{e}^{-\frac{x^2}{2}}}{(\gamma-2)(\gamma-1)\sqrt{\Gamma(\gamma)}} \left[\log(x^2) - \psi(\gamma) - \frac{\gamma-1}{x^2} + 1\right] \qquad \text{for} \quad \gamma > 2 \tag{2.7}$$

where $\psi$ is the digamma function [11]. Using (2.2) and (2.3), we have

$${}_4F_3(1,1,3,3;2,2,\gamma+1;1) = \frac{1}{4} \frac{\gamma(4\gamma^2 - 15\gamma + 13)}{(\gamma-1)(\gamma-2)(\gamma-3)} \qquad \gamma > 3$$

and therefore the perturbation expansion (1.12) follows immediately. These particular values of ${}_4F_3(1,1,3,3;2,2,\gamma+1;1)$ can be verified by means of the following lemma that extends the earlier identity

$${}_3F_2(a,b,c+1;d,c;z) = {}_2F_1(a,b;d;z) + \frac{ab}{cd} z\, {}_2F_1(a+1,b+1;d+1;z)$$

given by Luke [29]. The proof follows immediately by use of the series representation for the hypergeometric functions ${}_3F_2$ and ${}_2F_1$, as given by (1.14).

**Lemma 1.** *For* $|z| < 1$,

$$\begin{aligned} {}_4F_3(a,b,c+1,d+1;e,c,d;z) &= {}_2F_1(a,b;e;z) \\ &\quad + \frac{ab}{ec}\left(1 + \frac{c+1}{d}\right) z\, {}_2F_1(a+1,b+1;e+1;z) \\ &\quad + \frac{(a)_2(b)_2}{dc(e)_2} z^2\, {}_2F_1(a+2,b+2;e+2;z). \end{aligned} \tag{2.8}$$

*Further, in the case of* $|z| = 1$ *and* $e - a - b > 2$,

$$\begin{aligned} {}_4F_3(a,b,c+1,d+1;e,c,d;1) &= \frac{\Gamma(e)}{\Gamma(e-a)\Gamma(e-b)} \left[\Gamma(e-a-b) + \frac{ab}{c}\left(1 + \frac{c+1}{d}\right)\right. \\ &\quad \left. \times \Gamma(e-a-b-1) + \frac{(a)_2(b)_2}{dc}\Gamma(e-a-b-2)\right]. \end{aligned} \tag{2.9}$$

In the case of $\alpha = 6$, the first-order correction of the wavefunction reads [27, 28]

$$\phi_1(x) = \frac{1}{2\sqrt{2}} \frac{\Gamma(\gamma-3)}{\Gamma(\gamma)\sqrt{\Gamma(\gamma)}} x^{\gamma-1/2}\,\mathrm{e}^{-x^2/2} \left[\log(x^2) - \psi(\gamma) + \frac{3}{2} - \frac{\gamma-1}{x^2} - \frac{(\gamma-1)(\gamma-2)}{2x^4}\right] \tag{2.10}$$

consequently, from $\epsilon_2 = (\psi_0, x^{-6}\phi_1)$, we have for $\gamma > 5$

$$
{}_4F_3(1,1,4,4;2,2,\gamma+1;1) = \frac{\gamma}{18}\left(\frac{(\gamma-2)(\gamma-1)}{(\gamma-5)(\gamma-4)} + \frac{2(\gamma-1)}{(\gamma-4)} + \frac{(40-57\gamma+24\gamma^2-3\gamma^3)}{(\gamma-3)(\gamma-2)(\gamma-1)}\right). \tag{2.11}
$$

Therefore equation (1.8) takes the simpler form (1.13), as the result of (2.11). In order to extend (1.12) and (1.13) to the third-order perturbation correction, we need only use the expression $\epsilon_3 = (\phi_1, V\phi_1) - \epsilon_1(\phi_1, \phi_1)$, as mentioned in (2.2). Before we proceed with our calculations we shall first prove the following general result concerning the first-order correction of the wavefunction.

**Lemma 2.** *The first-order perturbation correction $\phi_1(x)$ of the exact solution of Hamiltonian (1.5), with arbitrary $\alpha$, satisfies the following normalization condition:*

$$
(\phi_1, \phi_1) = \frac{\alpha^2}{64\gamma}\frac{\Gamma^2\left(\gamma-\frac{\alpha}{2}\right)}{\Gamma^2(\gamma)}\,{}_5F_4\left(1,1,1,\frac{\alpha}{2}+1,\frac{\alpha}{2}+1;2,2,2,\gamma+1;1\right)
$$

*as long as $\alpha < \gamma + 2$.*

**Proof.** We note that, by comparing the expression for $\epsilon_3$ in (2.2) and (2.3), we find

$$
(\phi_1, \phi_1) = \sum_{i=1}^{\infty}\frac{|V_{0i}|^2}{(E_i - E_0)^2}.
$$

For the Hamiltonian (1.5), $V_{0i}$ is given by (2.5) and $E_i$ is given by (1.7); therefore, we have

$$
\begin{aligned}
(\phi_1, \phi_1) &= \frac{1}{16}\frac{\Gamma^2\left(\gamma-\frac{\alpha}{2}\right)}{\Gamma^2(\gamma)}\sum_{i=1}^{\infty}\frac{\left(\frac{\alpha}{2}\right)_i^2}{i^2\, i!(\gamma)_i} \\
&= \frac{1}{16}\frac{\Gamma^2\left(\gamma-\frac{\alpha}{2}\right)}{\Gamma^2(\gamma)}\sum_{i=0}^{\infty}\frac{\left(\frac{\alpha}{2}\right)_{i+1}^2}{(i+1)^2(i+1)!(\gamma)_{i+1}} \\
&= \frac{\alpha^2}{64\gamma}\frac{\Gamma^2\left(\gamma-\frac{\alpha}{2}\right)}{\Gamma^2(\gamma)}\sum_{i=0}^{\infty}\frac{(1)_i(1)_i(1)_i\left(\frac{\alpha}{2}+1\right)_i^2}{(2)_i(2)_i(2)_i(\gamma+1)_i}\frac{1}{i!} \\
&= \frac{\alpha^2}{64\gamma}\frac{\Gamma^2\left(\gamma-\frac{\alpha}{2}\right)}{\Gamma^2(\gamma)}\,{}_5F_4\left(1,1,1,\frac{\alpha}{2}+1,\frac{\alpha}{2}+1;2,2,2,\gamma+1;1\right)
\end{aligned}
$$

where we have used the Pochhammer identities $(a)_{n+1} = a(a+1)_n$, $(1)_n = n!$ and $(2)_n = (n+1)!$ (see (1.15)), and the series representation for the hypergeometric function ${}_5F_4$, as given by (1.14). □

Direct computations, using $\epsilon_3 = (\phi_1, x^{-4}\phi_1) - \epsilon_1(\phi_1, \phi_1)$ where $\phi_1$ is given by (2.7) and $\epsilon_1 = \frac{\Gamma(\gamma-2)}{\Gamma(\gamma)}$ leads, for $\alpha = 4$ and $\gamma > 4$, to

$$
E(\lambda, \alpha=4) = 2\gamma + \frac{\lambda}{(\gamma-1)(\gamma-2)} - \lambda^2\frac{4\gamma^2-15\gamma+13}{4(\gamma-1)^3(\gamma-2)^3(\gamma-3)} + \left\{\frac{16\gamma^5-175\gamma^4+742\gamma^3-1525\gamma^2+1520\gamma-590}{8(\gamma-4)(\gamma-3)^2(\gamma-2)^5(\gamma-1)^5}\right\}\lambda^3 + \cdots. \tag{2.12}
$$

For the case of $\alpha = 6$, the first-order correction of the wavefunction is given by (2.10). After some straightforward algebraic calculations, the ground-state perturbation expansion, up to the third order of $\lambda$ and valid for $\gamma > 7$, now reads

$$
E(\lambda, \alpha=6) = 2\gamma + \epsilon_1\lambda + \epsilon_2\lambda^2 + \epsilon_3\lambda^3 + \cdots \tag{2.13}
$$

**Table 1.** A comparison between the upper bounds for the Hamiltonian (1.5), for a wide range of values of $A = l(l+1)$ and $\lambda$, by formula (2.14) and the bounds $E_a^U$ obtained by Aguilera-Navarro *et al* [21]. Exact results $E$ found by the direct numerical solution of Schrödinger's equation are also presented.

| $\lambda$ | $l$ | $E_a^U$ | $E^U$ | $E$ |
|---|---|---|---|---|
| 0.001 | 3 | 9.000 114 279 82 | 9.000 114 279 12 | 9.000 114 279 12 |
| | 4 | 11.000 063 4908 | 11.000 063 4907 | 11.000 063 490 74 |
| | 5 | 13.000 040 4037 | 13.000 040 4036 | 13.000 040 403 64 |
| 0.01 | 3 | 9.001 142 268 25 | 9.001 142 199 48 | 9.001 142 199 40 |
| | 4 | 11.000 634 7955 | 11.000 634 7888 | 11.000 634 788 89 |
| | 5 | 13.000 404 0018 | 13.000 404 0006 | 13.000 404 000 60 |
| 0.1 | 3 | 9.011 370 328 09 | 9.011 364 261 69 | 9.011 364 026 18 |
| | 4 | 11.006 336 7394 | 11.006 336 1001 | 11.006 336 099 23 |
| | 5 | 13.004 036 5464 | 13.004 036 4325 | 13.004 036 432 52 |
| 1 | 3 | 9.109 013 250 38 | 9.109 311 262 10 | 9.108 658 607 52 |
| | 4 | 11.062 293 1434 | 11.062 249 2820 | 11.062 241 719 38 |
| | 5 | 13.040 025 4838 | 13.040 015 5515 | 13.040 015 183 06 |
| | 50 | 103.000 400 037 | 103.000 400 036 | 103.000 400 036 76 |

where

$$\epsilon_1 = \frac{\lambda}{(\gamma-1)(\gamma-2)(\gamma-3)}$$

$$\epsilon_2 = -\frac{\Gamma^2(-3+\gamma)}{8\Gamma^2(\gamma)}\left(\frac{(\gamma-2)(\gamma-1)}{(\gamma-5)(\gamma-4)} + \frac{2(\gamma-1)}{(\gamma-4)} + \frac{(40-3\gamma(19+(-8+\gamma)\gamma))}{(\gamma-3)(\gamma-2)(\gamma-1)}\right)$$

and $\epsilon_3 = \frac{I_1}{I_2}$, for

$$I_1 = 192\,088 - 655\,905\gamma + 945\,811\gamma^2 - 751\,923\gamma^3 + 360\,811\gamma^4 - 107\,151\gamma^5 + 19\,257\gamma^6 - 1917\gamma^7 + 81\gamma^8$$

$$I_2 = 8(\gamma-7)(\gamma-5)^2(\gamma-4)(\gamma-3)^5(\gamma-2)^5(\gamma-1)^5.$$

From a first reading of the articles by Sinanoğlu [30] (the main results of which are not affected by his false claim), or even the work of Morse and Feshbach [31] on perturbation theory, one understands that expressions (2.12) and (2.13) are upper bounds to the exact energy since all the odd-order energies would form upper bounds to the exact energy. This is not in fact true because $\epsilon_2$ in the general perturbation expansion (2.1) will always have a negative sign, thus not guaranteeing the upper bounds [32, 33]. However, it *is* possible to obtain a definite upper bound to the exact eigenvalue by means of the perturbation expansion. Thus

$$E(\lambda,\alpha) = E_0 + \epsilon_1\lambda + \frac{\epsilon_2\lambda^2 + \epsilon_3\lambda^3}{1+\lambda^2(\phi_1,\phi_1)} \tag{2.14}$$

where $(\phi_1, \phi_1)$ is given by lemma 2. The upper bound (2.14) can easily be demonstrated by applying the variational principle to the approximate wavefunction $\phi = \psi_0 + \lambda\phi_1$, where $\psi_0$ and $\phi_1$ satisfy the zero- and first-order perturbation equations

$$H_0\psi_0 = E_0\psi_0 \qquad (H_0 - E_0)\phi_1 = (E_1 - V)\psi_0. \tag{2.15}$$

In table 1, we compare the upper bounds obtained by means of (2.14) in the case of $\alpha = 4$ and those of Aguilera-Navarro and Koo obtained by variational analysis using appropriate trial functions. In the following section, we shall obtain the symmetric lower and upper bounds by the method of Burrows *et al* [12].

## 3. Lower and upper bounds

It is natural to ask: how small $\lambda$ should be for the perturbation expansions (2.12) and (2.13) to be valid? The question can be answered by studying upper and lower bounds to the eigenvalues. Based on the difference between the bounds we can infer a definite indication of the accuracy of truncated Rayleigh–Schrödinger perturbation series, such as (2.12) and (2.13). Wide bounds show that the truncated Rayleigh–Schrödinger perturbation series is suspect, while tight bounds demonstrate the high accuracy of the truncated expansion. For our purposes, the most suitable procedure developed for assessing the accuracy of a truncated perturbation expansion is due to Burrows *et al* [12]. A brief review of the method is presented here: for further details the reader is referred to the original article. Most derivations of bounds for eigenvalues of self-adjoint operators start from a consideration of positive definite function

$$(\mu(\phi,\epsilon),\mu(\phi,\epsilon)) = ([H-\epsilon]\phi,[H-\epsilon]\phi) = (H\phi,H\phi) - (\phi,H\phi)^2 + (\epsilon-(\phi,H\phi))^2 \geqslant 0 \tag{3.1}$$

where $H$ is the operator in question, $\epsilon$ is a positive parameter and $\phi$ is a suitably chosen (normalized) function. If we expand the normalized function $\phi$ in terms of the complete set of eigenfunctions $\{\phi_n\}$ of $H$ with eigenvalues $E_n(\lambda)$, $\phi = \sum_n a_n\phi_n$, $a_n = (\phi,\phi_n)$, $(\phi,\phi) = 1 = \sum_n a_n^2$, we can express the positive definite function in (3.1) as

$$(\mu(\phi,\epsilon),\mu(\phi,\epsilon)) = \sum_n a_n^2(E_n(\lambda)-\epsilon)^2 \geqslant 0.$$

Let us assume that we have picked the value of $\epsilon$ to lie closest to the value of the $i$th eigenvalue $E_i$, i.e.

$$(\mu(\phi,\epsilon),\mu(\phi,\epsilon)) = \sum_n a_n^2(E_n(\lambda)-\epsilon)^2 \geqslant (E_i(\lambda)-\epsilon)^2 \geqslant 0. \tag{3.2}$$

Combining (2.6) and (2.7), it can easily be seen that

$$f_-(\epsilon) \leqslant E_i(\lambda) \leqslant f_+(\epsilon) \tag{3.3a}$$

where

$$f_\pm(\epsilon) = \epsilon \pm \sqrt{\|H\phi\|^2 - (\phi,H\phi)^2 + (\epsilon-(\phi,H\phi))^2}. \tag{3.3b}$$

It is not hard to show that $f_\pm(\epsilon)$ is indeed a monotonic increasing function of $\epsilon$. This result will turn out to be useful in the following discussion. The bounds of Burrows *et al* follow [12] by setting

$$\mu(\phi,E_p(\lambda)) = [H_0+\lambda V - E_p(\lambda)]\phi \tag{3.4}$$

where

$$\phi = N_1(\psi_0+\lambda\phi_1) \qquad E_p(\lambda) = E_0 + \sum_{i=1}^{p}\lambda^i\epsilon_i \tag{3.5}$$

and, for all $p \leqslant 3$, $\psi_0$ and $\phi_1$ satisfy the zero- and first-order equations of the Rayleigh–Schrödinger perturbation theory (2.15). Further, the $\epsilon_i$, $i = 1, 2, 3$, are given by means of (2.2). Here, $N_1$ in equation (3.5) is a normalization constant for the truncated first-order expansion of the exact wavefunction:

$$N_1 = (1+\lambda^2(\phi_1,\phi_1))^{-1/2}.$$

If $\phi$ and $E_p(\lambda)$ were exact, $\mu = 0$. Thus we expect $\mu$ to be small if $\phi$ and $E_p(\lambda)$ are good approximations to the exact solutions. Consequently, a good test of the approximations (3.3*a*)–(3.3*b*) may be made by examining the value of the norm $\|\mu\| = \sqrt{\mu^2}$. Simple calculations, using (3.5) and (2.2), now give

**Table 2.** Eigenvalue bounds for different values of λ for the Hamiltonian $H = -\frac{d^2}{dx^2} + x^2 + \frac{12}{x^2} + \frac{\lambda}{x^4}$. The underlined values are the optimal bounds according to inequality (3.10).

| | $\epsilon_1$ | | $\epsilon_2$ | | $\epsilon_3$ | |
|---|---|---|---|---|---|---|
| λ | $E_L$ | $E^U$ | $E_L$ | $E^U$ | $E_L$ | $E^U$ |
| 0.001 | <u>9.000 114 234</u> | 9.000 114 334 | 9.000 114 231 | <u>9.000 114 327</u> | 9.000 114 231 | 9.000 114 327 |
| 0.01 | <u>9.001 138 022</u> | 9.001 147 691 | 9.001 137 408 | <u>9.001 146 987</u> | 9.001 137 409 | 9.001 146 989 |
| 0.1 | <u>9.010 945 111</u> | 9.011 912 031 | 9.010 883 476 | <u>9.011 841 809</u> | 9.010 885 097 | 9.011 843 425 |
| 1 | <u>9.065 963 521</u> | 9.162 607 906 | 9.059 599 522 | <u>9.155 786 288</u> | 9.061 245 282 | 9.157 377 241 |

$$\|\mu(\phi, E_1(\lambda))\| = N_1\lambda^2(\phi_1, (V-\epsilon_1)^2\phi_1)^{1/2} \tag{3.6}$$

$$\|\mu(\phi, E_2(\lambda))\| = \left\{\|\eta(\phi, E_1(\lambda))\|^2 + \lambda^4\epsilon_2\left\{\epsilon_2 - 2N_1^2(\epsilon_2 + \lambda\epsilon_3)\right\}\right\}^{1/2} \tag{3.7}$$

and

$$\|\mu(\phi, E_3(\lambda))\| = \left\{\|\eta(\phi, E_2(\lambda))\|^2 + \lambda^4\left\{2\lambda^3\epsilon_2\epsilon_3\left(1 - N_1^2\right) - \lambda^2(1+\lambda^2)N_1^2\epsilon_3^2 + \lambda^4\epsilon_3^2\right\}\right\}^{1/2} \tag{3.8}$$

where we have reproduced the formulae of Burrows *et al* [12] for computational convenience. In this case, (3.3*a*) implies

$$f_-(E_p(\lambda)) \leqslant E(\lambda) \leqslant f_+(E_p(\lambda)) \tag{3.9a}$$

where

$$f_\pm(E_p(\lambda)) = E_p(\lambda) \pm \|\mu(\phi, E_p(\lambda))\| \qquad \text{for} \quad p = 1, 2, 3. \tag{3.9b}$$

The only new integral (beyond the usual integrals of Rayleigh–Schrödinger perturbation series) is seen to be $(\phi_1|(V-\epsilon_1)^2\phi_1)$ which restricts the value of $\gamma$, for example in the case of $\alpha = 4$, to be greater than 4 even if we have used the first-order approximation $\epsilon_1$ (for which $\gamma > 2$ is sufficient). This is, of course, due to the bound's dependence on $\epsilon_3$ which required $\gamma > 4$. The result in this case, however, is very useful [23, 34] when the radial Schrödinger equation is characterized by *large* angular momenta $l$. For $\gamma = 4.5$ (i.e. $A = 12$ or $l = 3$ for $A = l(l+1)$) and $\lambda = 0.001$, the first-order perturbation correction yields 9.000 114 285 with error bounds of $\pm 4.8346 \times 10^{-8}$. The second-order perturbation correction yields 9.000 114 279 with error bounds of $\pm 4.7879 \times 10^{-8}$; while $\epsilon_3$ yields 9.000 114 279 with an upper bound of 9.000 114 327 and a lower bound of 9.000 114 231. Now, for any fixed $\phi$, the bounding functions $f_\pm(E_p(\lambda))$ are easily shown to be monotonic increasing functions of $E_p(\lambda)$, $p = 1, 2, 3$, as we indicated above. Consequently the optimal bound for the set $\{E_1(\lambda) = E_0 + \lambda\epsilon_1, E_2(\lambda) = E_0 + \lambda\epsilon_1 + \lambda^2\epsilon_2, E_3(\lambda) = E_0 + \lambda\epsilon_1 + \lambda^2\epsilon_2 + \lambda^3\epsilon_3\}$ is indeed given, for $\lambda < \frac{|\epsilon_2|}{\epsilon_3}$, by

$$f_-(E_1(\lambda)) \leqslant E(\lambda) \leqslant f_+(E_2(\lambda)). \tag{3.10}$$

The inequality $\lambda < \frac{|\epsilon_2|}{\epsilon_3}$ allows us to order the approximated eigenvalues as $E_1(\lambda) > E_3(\lambda) > E_2(\lambda)$, for the sign of $\epsilon_2$ is always negative and the sign of $\epsilon_3$ is positive for moderate values of $\lambda$. In table 2, we have verified these results by obtaining upper and lower bounds for the eigenvalues by means of (3.6)–(3.8); underlined values are the optimal bounds. Similar bounds can be obtained for the case of $\alpha = 6$ by using (2.13). Although, the upper bounds obtained by this method are less accurate than the upper bounds obtained by means of (2.14), the advantage of this method is the symmetric lower and upper bounds available through (3.9).

## 4. Conclusions and some remarks

The main results of this paper are concrete upper- and lower-bound formulae (2.14), (3.9) and (3.10). There are many variational methods available to solve the eigenvalue problem for the Hamiltonian (1.5), however they provide only upper bounds and usually no information is available concerning the accuracy of the method other than comparison with numerical solutions of the Schrödinger equation in question. Furthermore, for very small values of the parameter $\lambda$, variational methods are usually slow and a large number of matrix elements are needed to obtain sufficient accuracy. We have presented upper and lower bounds for such situations which, as tables 1 and 2 indicate, provide excellent results for very small values of $\lambda$. Although, the techniques used to produce the present results are standard, the ability of these techniques to generate explicit bounds is a consequence of our pervious achievements, yielding concrete forms for the first-order perturbation corrections of the wavefunctions.

Apart from the upper and lower bounds obtained, there are also some interesting results concerning closed-form sums for double infinite series that follow directly from this work. It is clear from (2.2) and (2.3) that

$$\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{V_{0n}V_{nm}V_{m0}}{(E_0-E_n)(E_0-E_m)} = (\phi_1, V\phi_1) \tag{4.1}$$

where $V_{nm}, n = 1, 2, \ldots, m = 1, 2, \ldots,$ are given by (2.4). We will now look at the cases $\alpha = 2, 4, 6, \ldots$. Similar results can be obtained for the cases of $\alpha = 1, 3, 5, \ldots,$ by means of the first-order corrections for the wavefunctions given previously [27, 28]; however, the calculations will be more involved for such cases. For $\alpha = 2$, we know that the matrix elements (i.e. from (2.4)) read

$$V_{nm} = \begin{cases} (-1)^{n+m}\dfrac{\Gamma(\gamma-1)}{\Gamma(\gamma)}\sqrt{\dfrac{m!(\gamma)_n}{n!(\gamma)_m}} & \text{if} \quad m \geqslant n \\[2ex] (-1)^{n+m}\dfrac{\Gamma(\gamma-1)}{\Gamma(\gamma)}\sqrt{\dfrac{n!(\gamma)_m}{m!(\gamma)_n}} & \text{if} \quad n \geqslant m. \end{cases} \tag{4.2}$$

On the other hand, the first-order correction of the wavefunction in this case reads [27, 28]

$$\phi_1(x) = \frac{1}{\sqrt{2}}\frac{x^{\gamma-\frac{1}{2}}\,\mathrm{e}^{-\frac{x^2}{2}}}{(\gamma-1)\sqrt{\Gamma(\gamma)}}\left[\log(x) - \frac{1}{2}\psi(\gamma)\right] \qquad \text{for} \quad \gamma > 1. \tag{4.3}$$

Consequently, the following results follow immediately.

**Lemma 3.** *For $\gamma > 1$ and $V_{nm}$ as given by (4.2), we have*

$$\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{V_{0n}V_{nm}V_{m0}}{16nm} = \frac{1}{8(\gamma-1)^5} + \frac{\psi^{(1)}(\gamma)}{16(\gamma-1)^3} \tag{4.4}$$

*where $\psi^{(1)}(\gamma)$ is the first derivative of the digamma functions.*

The proof of this lemma is obtained by calculating the inner product of the right-hand side of (4.1) by means of (4.3) for $0 \leqslant x < \infty$, where $V(x) = x^{-2}$ and

$E_n = 4n + 2\gamma$ ($n = 0, 1, 2, \ldots$). For the case $\alpha = 4$ and $\gamma > 2$, the matrix elements (2.4) read

$$V_{nm} = \begin{cases} (-1)^{n+m}\dfrac{\Gamma(\gamma-2)}{\Gamma(\gamma+1)}\sqrt{\dfrac{m!(\gamma)_n}{n!(\gamma)_m}}[\gamma(m-n+1)+2n] & \text{if} \quad m \geqslant n \\ (-1)^{n+m}\dfrac{\Gamma(\gamma-2)}{\Gamma(\gamma+1)}\sqrt{\dfrac{n!(\gamma)_m}{m!(\gamma)_n}}[\gamma(n-m+1)+2m] & \text{if} \quad n \geqslant m. \end{cases} \tag{4.5}$$

On the other hand, the first-order corrections of the wavefunction for this case are given by (2.7). Therefore (4.1) leads to the following results.

**Lemma 4.** *For $\gamma > 4$ and $V_{nm}$ as given by (4.5), we have*

$$\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{V_{0n}V_{nm}V_{m0}}{16nm} = \frac{-820+1954\gamma-1753\gamma^2+694\gamma^3-90\gamma^4-12\gamma^5+3\gamma^6}{16(\gamma-4)(\gamma-3)^2(\gamma-2)^5(\gamma-1)^5} + \frac{\psi^{(1)}(\gamma)}{16(\gamma-2)^3(\gamma-1)^3} \tag{4.6}$$

*where $\psi^{(1)}(\gamma)$ is the first derivative of the digamma functions.*

As the final case that we illustrate, namely $\alpha = 6$ and $\gamma > 3$, we point to the fact that equation (2.4) lets us deduce

$$V_{nm} = \begin{cases} (-1)^{n+m}\dfrac{\Gamma(\gamma-3)}{2\Gamma(\gamma+2)}\sqrt{\dfrac{m!(\gamma)_n}{n!(\gamma)_m}}[(2+m)(1+m)\gamma(\gamma+1) \\ -2n(1+m)(\gamma-3)(\gamma+1)-n(1-n)(\gamma-2)(\gamma-3)] & \text{if} \quad m \geqslant n \\ (-1)^{n+m}\dfrac{\Gamma(\gamma-3)}{2\Gamma(\gamma+2)}\sqrt{\dfrac{n!(\gamma)_m}{m!(\gamma)_n}}[(2+n)(1+n)\gamma(\gamma+1) \\ -2m(1+n)(\gamma-3)(\gamma+1)-m(1-m)(\gamma-2)(\gamma-3)] & \text{if} \quad n \geqslant m. \end{cases} \tag{4.7}$$

where the first-order correction for the wavefunction is now given by (2.10). Therefore, by means of (4.1), we conclude with the following lemma.

**Lemma 5.** *For $\gamma > 7$ and $V_{nm}$ as given by (4.7), we have*

$$\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{V_{0n}V_{nm}V_{m0}}{16nm} = \frac{I_1}{I_2} + \frac{\psi^{(1)}}{16(\gamma-3)^3(\gamma-2)^3(\gamma-1)^3} \tag{4.8}$$

*where*

$$I_1 = 522\,652 - 1717\,440\gamma + 2371\,931\gamma^2 - 1785\,046\gamma^3 + 792\,061\gamma^4 - 206\,964\gamma^5 + 28\,725\gamma^6 - 1158\gamma^7 - 169\gamma^8 + 16\gamma^9$$

*and*

$$I_2 = 32(\gamma-7)(\gamma-5)^2(\gamma-4)(\gamma-3)^5(\gamma-2)^5(\gamma-1)^5$$

*where $\psi^{(1)}(\gamma)$ is the first derivative of the digamma function.*

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