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Perturbation expansions for the spiked harmonic oscillator and related series involving the gamma function

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Abstract. We study weak-coupling perturbation expansions for the ground-state energy of the Hamiltonian with the generalized spiked harmonic oscillator potential $V(x) = Bx^2 + \frac{A}{x^2} + \frac{\lambda}{x^\alpha}$, and also for the bottoms of the angular-momentum subspaces labelled by $l = 0, 1, \ldots$, in N dimensions corresponding to the spiked harmonic oscillator potential $V(x) = x^2 + \frac{\lambda}{x^\alpha}$, where α is a real positive parameter. A method of Znojil (Znojil M 1993 *J. Math. Phys.* **34** 4914) is then applied to obtain closed-form expressions for the sums of some infinite series whose terms involve ratios and products of gamma functions.

1. Introduction

The spiked harmonic oscillator Hamiltonian defined by

$$H = -\frac{d^2}{dx^2} + x^2 + \frac{\lambda}{x^\alpha} \qquad \alpha < \tfrac{5}{2} \qquad x \in [0, \infty) \tag{1.1}$$

where the positive parameter λ measures the strength of the singular term, has been the subject of intensive study [1–3]. Aguilera-Navarro and Guardiola [1], employed a resummation technique to obtain a weak-coupling perturbation expansion for the ground-state energy of the Hamiltonian (1.1), using standard perturbation theory up to second order. The Hamiltonian (1.1) is first written $H = H_0 + \lambda V$; then, using the odd-parity solutions of the one-dimensional harmonic oscillator $\psi_n(x) = |n\rangle$ satisfying the Dirichlet boundary condition $\psi(0) = 0$, and the unperturbed energies $E_n = 3 + 4n$, $n = 0, 1, 2, \ldots$, they found that the weak-coupling expansion for the ground state of H to the second order in V becomes

$$E = E_0 + \lambda\langle 0|x^{-\alpha}|0\rangle + \lambda^2 \sum_{n\geqslant 1} \frac{|\langle 0|x^{-\alpha}|n\rangle|^2}{E_0 - E_n} + \cdots \qquad \alpha < \tfrac{5}{2} \tag{1.2}$$

where $\langle 0|x^{-\alpha}|n\rangle$ is given by

$$\langle 0|x^{-\alpha}|n\rangle = \frac{(-2)^n}{\sqrt{(2n+1)!}} \frac{\Gamma(\frac{3-\alpha}{2})\Gamma(\frac{\alpha}{2} + n)}{\Gamma(\frac{3}{2})\Gamma(\frac{\alpha}{2})} \qquad n = 0, 1, \ldots. \tag{1.3}$$

In their pertubation treatment, Aguilera-Navarro and Guardiola construct a function F, expressed in terms of a particular form of the Gauss hypergeometric series; the function F was found to be useful for obtaining analytic approximations for the ground-state energy of the for the 'non-supersingular' cases: $\alpha = \frac{1}{2}$, $\alpha = 1$ and $\alpha = \frac{3}{2}$. They also provided a weak-coupling expression valid for the case $\alpha = 2$. Estévez-Bretòn *et al* [2] derived an exact analytical result,

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by using the function F, valid for the special case $\alpha = 2$. Later Znojil [3] derived the same result by an elegant and economical method. It is perhaps worth noting here that in all these works, although the conclusions and the results were correct, there remained an error in the F formula, equation (14) in [1], deduced by Aguilera-Navarro and Guardiola, which should read

$$F = \frac{1}{8(\frac{\alpha}{2}-1)^2}\left[{}_2F_1\left(\frac{\alpha}{2}-1, \frac{\alpha}{2}-1; \frac{1}{2}; 1\right) - 1 - 2\left(\frac{\alpha}{2}-1\right)^2\right].$$

In section 2 of the present paper we generalize the weak-coupling expansion (1.2) to study the generalized spiked harmonic oscillator Hamiltonian

$$H \equiv H_0 + \lambda V = -\frac{d^2}{dx^2} + Bx^2 + \frac{A}{x^2} + \frac{\lambda}{x^\alpha} \qquad \alpha < \tfrac{5}{2} \quad x \in [0, \infty) \tag{1.4}$$

where λ and α are positive parameters. We show that the weak-coupling expansion, in this case, is given by

$$E = 2\sqrt{B}\gamma + B^{\frac{\alpha}{4}}\frac{\Gamma(\gamma-\frac{\alpha}{2})}{\Gamma(\gamma)}\lambda - \lambda^2\frac{B^{\frac{\alpha-1}{2}}\alpha^2}{16\gamma}\frac{\Gamma^2(\gamma-\frac{\alpha}{2})}{\Gamma^2(\gamma)}$$
$$\times {}_4F_3\left(1, 1, \frac{\alpha}{2}+1, \frac{\alpha}{2}+1; \gamma+1, 2, 2; 1\right) + \cdots$$

where $\gamma = 1 + \frac{1}{2}\sqrt{1+4A}$. This expression is valid for all values of $\alpha < \gamma + 1$, including $\alpha = 2$. This formula allows us to obtain perturbation expansions for (1.1) and (1.4) valid for the bottoms of the angular-momentum subspaces labelled by $l = 0, 1, \ldots$ in N dimensions. In section 3, we adopt the constructive approach of Aguilera-Navarro and Guardiola to generalize the function F, which we then use to obtain a sum for the infinite series

$$\sum_{n\geqslant 1}\frac{(\frac{\alpha}{2})_n^2}{4n(n+1)(\gamma)_n n!}.$$

In section 4, by employing Znojil's technique [3], our generalization turns out to be useful for obtaining closed-form sums for other interesting infinite series whose terms involve ratios and products of gamma functions.

2. Weak-coupling expansions

Recently, we have obtained expressions [4] for the singular-potential integrals $\langle m|x^{-\alpha}|n\rangle$ of the Hamiltonian (1.4) using the Gol'dman and Krivchenkov eigenfunctions [5]

$$\psi_n(x) \equiv |n\rangle = C_n x^{\frac{1}{2}(1+\sqrt{1+4A})} e^{-\frac{1}{2}\sqrt{B}x^2} {}_1F_1\left(-n, 1+\tfrac{1}{2}\sqrt{1+4A}; \sqrt{B}x^2\right)$$
$$C_n^2 = \frac{2B^{\frac{1}{2}+\frac{1}{4}\sqrt{1+4A}}\Gamma\left(n+1+\frac{1}{2}\sqrt{1+4A}\right)}{n!\left[\Gamma\left(1+\frac{1}{2}\sqrt{1+4A}\right)\right]^2} \qquad n = 0, 1, 2, \ldots \tag{2.1}$$

where ${}_1F_1$ is the confluent hypergeometric function [9]

$${}_1F_1(a, b; z) = \sum_k \frac{(a)_k z^k}{(b)_k k!} \qquad (a)_k = a(a+1)\ldots(a+k-1) = \frac{\Gamma(a+k)}{\Gamma(a)} \tag{2.2}$$

and the exact eigenenergies $E_n = \sqrt{B}(4n + 2 + \sqrt{1+4A})$, $n = 0, 1, 2, \ldots$, for the singular Hamiltonian

$$H_0 = -\frac{d^2}{dx^2} + Bx^2 + \frac{A}{x^2} \qquad B > 0 \qquad A \geqslant 0 \qquad x \in [0, \infty). \tag{2.3}$$

Hall *et al* [4] found, for $\alpha < 2\gamma$, that the matrix elements $\langle m|x^{-\alpha}|n\rangle$ are given by

$$\langle m|x^{-\alpha}|n\rangle = (-1)^{n+m} B^{\alpha/4}\sqrt{\frac{\Gamma(\gamma+m)}{n!m!\Gamma(\gamma+n)}} \times \sum_{k=0}^{m}(-1)^k \binom{m}{k}\frac{\Gamma(k+\gamma-\frac{\alpha}{2})\Gamma(\frac{\alpha}{2}-k+n)}{\Gamma(k+\gamma)\Gamma(\frac{\alpha}{2}-k)} \qquad \gamma = 1+\tfrac{1}{2}\sqrt{1+4A} \tag{2.4}$$

in which each element has a factor which is a polynomial of degree $m+n$ in α. The relevant matrix elements $\langle 0|x^{-\alpha}|n\rangle$ are given [4] by

$$\langle 0|x^{-\alpha}|n\rangle = (-1)^n B^{\alpha/4}\sqrt{\frac{\Gamma(\gamma)}{n!\Gamma(\gamma+n)}}\frac{\Gamma(\gamma-\frac{\alpha}{2})\Gamma(\frac{\alpha}{2}+n)}{\Gamma(\gamma)\Gamma(\frac{\alpha}{2})} \qquad n = 0, 1, 2, \ldots. \tag{2.5}$$

Thus, writing (1.4) as $H = H_0 + \lambda V$ and using the standard perturbation theory to the second order, we find that the weak-coupling expansion (1.2) now reads

$$E = 2\sqrt{B}\gamma + B^{\frac{\alpha}{4}}\frac{\Gamma(\gamma-\frac{\alpha}{2})}{\Gamma(\gamma)}\lambda - \lambda^2 B^{\frac{\alpha-1}{2}}\frac{\Gamma^2(\gamma-\frac{\alpha}{2})}{\Gamma^2(\gamma)}\sum_{n\geqslant 1}\frac{(\frac{\alpha}{2})_n^2}{4n(\gamma)_n n!} + \cdots \qquad \alpha < \gamma+1 \tag{2.6}$$

where $\gamma = 1+\frac{1}{2}\sqrt{1+4A}$. We observe that the ratio of the nth and $(n+1)$th terms of the sum in the coefficient of λ^2 in (2.6) is

$$\frac{\langle 0|x^{-\alpha}|n\rangle^2/(E_n-E_0)}{\langle 0|x^{-\alpha}|n+1\rangle^2/(E_{n+1}-E_0)} = 1 + \frac{\gamma+2-\alpha}{n} + \mathrm{o}\left(\frac{1}{n^2}\right) \qquad \text{as} \quad n\to\infty$$

so that, by Raabe's test [6], this sum is convergent for $\alpha < \gamma+1$. The expressions (1.2) and (2.6) are accurate for λ small compared to unity. It is interesting that the sum of the infinite series in the λ^2 coefficient can be computed exactly for arbitrary values of α and γ satisfying $\alpha < \gamma+1$. We express the sum in terms of the generalized hypergeometric functions ${}_pF_q$ defined [7] by

$${}_pF_q(\alpha_1, \alpha_2, \ldots, \alpha_p; \beta_1, \beta_2, \ldots, \beta_q; z) = \sum_{n=0}^{\infty}\frac{(\alpha_1)_n(\alpha_2)_n\ldots(\alpha_p)_n}{(\beta_1)_n(\beta_2)_n\ldots(\beta_q)_n}\frac{z^n}{n!}. \tag{2.7}$$

Indeed, the sum in the λ^2 coefficient implies

$$\begin{aligned}\sum_{n\geqslant 1}\frac{(\frac{\alpha}{2})_n^2}{4n(\gamma)_n n!} &= \sum_{n\geqslant 1}\frac{(n-1)!(\frac{\alpha}{2})_n^2}{4(\gamma)_n(n!)^2}\\ &= \frac{1}{4}\sum_{n=0}\frac{(n!)^2(\frac{\alpha}{2})_{n+1}^2}{((n+1)!)^2(\gamma)_{n+1}n!}\\ &= \frac{\alpha^2}{16\gamma}\sum_{n=0}\frac{(1)_n^2(\frac{\alpha}{2}+1)_n^2}{(2)_n^2(\gamma+1)_n n!}\\ &= \frac{\alpha^2}{16\gamma}\,{}_4F_3\left(1, 1, \frac{\alpha}{2}+1, \frac{\alpha}{2}+1; \gamma+1, 2, 2; 1\right)\end{aligned} \tag{2.8}$$

where we have used the Pochhammer identities $(z)_{n+1} = z(z+1)_n$ and $n! = (1)_n$. This expression can easily be computed for arbitrary values of $\alpha < \gamma+1$ by the use, for example, of Mathematica. The weak-coupling expansion (2.6) now reads

$$E = 2\sqrt{B}\gamma + B^{\frac{\alpha}{4}}\frac{\Gamma(\gamma-\frac{\alpha}{2})}{\Gamma(\gamma)}\lambda - \lambda^2\frac{B^{\frac{\alpha-1}{2}}\alpha^2}{16\gamma}\frac{\Gamma^2(\gamma-\frac{\alpha}{2})}{\Gamma^2(\gamma)} \times {}_4F_3\left(1,1,\frac{\alpha}{2}+1,\frac{\alpha}{2}+1;\gamma+1,2,2;1\right)+\cdots. \tag{2.9}$$

The results of Aguilera-Navarro and Guardiola for the special case $B = 1$, $A = 0$ or $\gamma = \frac{3}{2}$, and for the values of $\alpha = \frac{1}{2}$, $\alpha = 1$, $\alpha = \frac{3}{2}$ and $\alpha = 2$ follow immediately without the necessity of special treatment for the case of $\alpha = 2$ as suggested before by many workers in the field [1–3]. The expression (2.9) can be further generalized to apply 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 [8] to replace A with $A \to A + (l + \frac{1}{2}(N-1))(l + \frac{1}{2}(N-3))$. For the spiked harmonic oscillator potential (1.1), we set $A = 0$ or we replace γ with $l + \frac{N}{2}$ to obtain a weak-coupling expansion valid for the bottoms of the angular-momentum subspaces in N dimensions.

3. The F function

Although our results in section 2 cover all the cases for $\alpha < \frac{5}{2}$ for the Hamiltonians (1.1) and (1.4) the constructive approach of Aguilera-Navarro and Guardiola allows us to obtain more sums of infinite series involving gamma functions. We first generalize the function F as introduced in [1] (we also point out the error in the F formula there). If we denote the sum in the λ^2 coefficient of equation (2.6) by

$$G = \sum_{n\geqslant 1}\frac{(\frac{\alpha}{2})_n^2}{4n(\gamma)_n n!} \tag{3.1}$$

and compare this with the sum

$$F = \sum_{n\geqslant 1}\frac{(\frac{\alpha}{2})_n^2}{4(n+1)(\gamma)_n n!} \tag{3.2}$$

we see that G and F are related by the expression

$$G = F + \sum_{n\geqslant 1}\frac{(\frac{\alpha}{2})_n^2}{4n(n+1)(\gamma)_n n!}. \tag{3.3}$$

The new expression for the sum thus obtained will be easier to approximate since fewer terms will be required for a given accuracy. Moreover, using the Pochhammer identity $(z)_{n+1} = z(z+1)_n$, we note that F can be written in terms of a special form of the Gauss hypergeometric function [9]

$${}_2F_1(a,b;c;z) = \sum_{n=0}\frac{(a)_n(b)_n}{(c)_n}\frac{z^n}{n!} \tag{3.4}$$

(with a circle of convergence $|z| = 1$) as

$$F = \frac{(\gamma-1)}{4(\frac{\alpha}{2}-1)^2}\left[{}_2F_1\left(\frac{\alpha}{2}-1,\frac{\alpha}{2}-1;\gamma-1;1\right)-1-\frac{(\frac{\alpha}{2}-1)^2}{(\gamma-1)}\right]. \tag{3.5}$$

This generalizes the weak-coupling expansion derived by Aguilera-Navarro and Guardiola to study equation (1.4) for $\alpha < \gamma+1$. However, we should note here the correct form of function F of the case $\gamma = \frac{3}{2}$ or $A = 0$, that is

$$F = \frac{1}{8(\frac{\alpha}{2}-1)^2}\left[{}_2F_1\left(\frac{\alpha}{2}-1,\frac{\alpha}{2}-1;\frac{1}{2};1\right)-1-2\left(\frac{\alpha}{2}-1\right)^2\right] \tag{3.6}$$

not as quoted in [1–3]. Equations (2.8) and (3.5) can be used now to obtain a sum for the infinite series

$$\sum_{n\geqslant 1} \frac{(\frac{\alpha}{2})_n^2}{4n(n+1)(\gamma)_n n!} = \frac{\alpha^2}{16\gamma}\, {}_4F_3\left(1, 1, \frac{\alpha}{2}+1, \frac{\alpha}{2}+1; \gamma+1, 2, 2; 1\right)$$
$$-\frac{(\gamma-1)}{4(\frac{\alpha}{2}-1)^2}\left[{}_2F_1\left(\frac{\alpha}{2}-1, \frac{\alpha}{2}-1; \gamma-1; 1\right) - 1 - \frac{(\frac{\alpha}{2}-1)^2}{(\gamma-1)}\right] \tag{3.7}$$

valid for $\alpha \neq 2$. For the special limit $\alpha = 2$, the expression (3.5) has no meaning. However, the sum in the λ^2 coefficient of (2.6) converges and follows from (2.8) by setting $\alpha = 2$. Indeed, in this case, the sum in (2.6) becomes

$$\sum_{n\geqslant 1} \frac{(1)_n^2}{4n(\gamma)_n n!} = \sum_{n\geqslant 1} \frac{(n-1)!}{4(\gamma)_n} = \sum_{n=0} \frac{(1)_n^2}{4(\gamma)_{n+1} n!} = \frac{1}{4\gamma}\, {}_2F_1(1, 1; \gamma+1; 1) \tag{3.8}$$

which follows immediately from (2.8). The Gauss hypergeometric function ${}_2F_1(1, 1; \gamma+1; 1)$ can be evaluated using the identity [9]

$${}_2F_1(a, b, c; 1) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} \qquad c-a-b>0 \qquad c>b>0 \tag{3.9}$$

to obtain

$$\sum_{n\geqslant 1} \frac{(1)_n^2}{4n(\gamma)_n n!} = \frac{1}{4(\gamma-1)} \qquad \gamma > 1. \tag{3.10}$$

Thus, for the case $\alpha = 2$, the weak-coupling expansion (2.9) becomes

$$E(\alpha=2) = 2\sqrt{B}\gamma + \frac{\sqrt{B}}{(\gamma-1)}\lambda - \frac{\sqrt{B}}{4(\gamma-1)^3}\lambda^2 + \cdots \qquad \gamma > 1 \tag{3.11}$$

and finally, for $B = 1$, $A = 0$ or $\gamma = \frac{3}{2}$, we obtain

$$E(\alpha=2) = 3 + 2\lambda - 2\lambda^2 + \cdots \tag{3.12}$$

as we expect.

4. More closed-form sums of infinite series

For the special limiting case $\alpha \to 2$, we introduce a parameter $\epsilon = \frac{\alpha}{2} - 1$, which will be chosen to approach zero. The function F, as given by (3.5), becomes in this limit

$$\lim_{\epsilon\to 0} F = \frac{(\gamma-1)}{4} \lim_{\epsilon\to 0} \epsilon^{-2}[{}_2F_1(\epsilon, \epsilon, \gamma-1, 1) - 1] - \frac{1}{4}. \tag{4.1}$$

Using the series expansion of the Gauss hypergeometric function (3.4), equation (4.1) can be written, using $\Gamma(z+1) = z\Gamma(z)$, as

$$\lim_{\epsilon\to 0} F = \frac{1}{4}\sum_{n=0}^{\infty} \frac{\Gamma(n)\Gamma(\gamma)}{n\Gamma(n+\gamma-1)} - \frac{1}{4}. \tag{4.2}$$

Some results similar to equations (4.1) and (4.2), were first published, without detailed proofs, by Mitchell [11]. Now, using the identity (3.9), equation (4.1) can be rewritten as

$$\lim_{\epsilon\to 0} F = \frac{(\gamma-1)}{4} \lim_{\epsilon\to 0} \epsilon^{-2}\left[\frac{\Gamma(\gamma-1)\Gamma(\gamma-1-2\epsilon)}{\Gamma^2(\gamma-1-\epsilon)} - 1\right] - \frac{1}{4}. \tag{4.3}$$

Now employing Znojil's method [3], we can obtain closed form sums for other infinite series involving gamma functions. Indeed, the Maclaurin expansion of the gamma function

$$\Gamma(c+x) = \Gamma(c)\{1 + x\psi(c) + \tfrac{1}{2}[\psi^2 + \psi^{(1)}(c)] + \cdots\} \tag{4.4}$$

where $\psi(c)$ and $\psi^{(n)}(c)$, $n \geqslant 1$, are the digamma and the polygamma functions [10], respectively. We can show, after expanding the gamma functions in (4.3) and employing multiplication and division of polynomials, that equation (4.4) can be written as

$$\lim_{\epsilon\to 0} F = \frac{(\gamma-1)}{4}\psi^{(1)}(\gamma-1) - \frac{1}{4} \tag{4.5}$$

where $\psi^{(n)}(z)$ are the polygamma functions. Comparing (4.2) and (4.5), we have

$$\sum_{n=1}^{\infty} \frac{\Gamma(n)\Gamma(\gamma-1)}{n\Gamma(n+\gamma-1)} = \psi^{(1)}(\gamma-1) \qquad \gamma > 1 \tag{4.6}$$

where $\psi^{(1)}(z)$ is the trigamma function [7]. For the purpose principally of verification we now note some special cases. For $\gamma = 2$

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6} \tag{4.7}$$

and for $\gamma - 1 = m \geqslant 2$ positive integer, we find

$$\sum_{n=1}^{\infty} \frac{\Gamma(n)\Gamma(m)}{n\Gamma(n+m)} = \frac{\pi^2}{6} - \sum_{k=2}^{m} \frac{1}{(k-1)^2} \tag{4.8}$$

by using the recurrence relation

$$\psi^{(n)}(z+1) = \psi^{(n)}(z) + (-1)^n n! z^{-n-1}.$$

Further, for $\gamma = \frac{3}{2}$

$$\sum_{n=1}^{\infty} \frac{\Gamma(n)\Gamma(\frac{1}{2})}{n\Gamma(n+\frac{1}{2})} = \frac{\pi^2}{2} \tag{4.9}$$

and

$$\sum_{n=1}^{\infty} \frac{\Gamma(n)\Gamma(mz)}{n\Gamma(n+mz)} = \frac{1}{m^2} \sum_{k=0}^{m-1} \psi^{(1)}\left(z + \frac{k}{m}\right). \tag{4.10}$$

Finally, we can now have a finite sum for the infinite series (3.7) for the case $\alpha = 2$ and $\gamma > 1$,

$$\sum_{n\geqslant 1} \frac{(1)_n^2}{4n(n+1)(\gamma)_n n!} = \frac{1}{4\gamma}\,{}_2F_1(1,1;\gamma+1;1) - \frac{\gamma-1}{4}\psi^{(1)}(\gamma-1) + \frac{1}{4}. \tag{4.11}$$

5. Conclusion

We have obtained a compact weak-coupling expansion (2.9) for eigenvalues of the spiked harmonic oscillator Hamiltonian. Our expansion extends the earlier work of Aguilera-Navarro and Guardiola for $\gamma \neq \frac{3}{2}$, and it allows for arbitrary spatial dimension N and also, for $N \geqslant 2$, arbitrary orbital angular-momentum ℓ. Moreover, with the closed-form expressions we have been able to provide for the coefficient of the λ^2 term, the new expansion is easier to handle and calculate with, even at or near to the special value $\alpha = 2$. These analytic expressions describe approximately how the eigenvalues depend on all the parameters in the Hamiltonian. Such formulas are complementary to data obtained with the aid of a computer; moreover, they are useful in guiding a procedure that searches for very accurate numerical eigenvalues. As a byproduct of this work, we have been led to some simple closed forms for a variety of interesting infinite series involving sums and ratios of gamma functions.

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