Variational analysis for a generalized spiked harmonic oscillator

2000 J. Phys. A: Math. Gen. 33 569

(http://iopscience.iop.org/0305-4470/33/3/310)

J. Phys. A: Math. Gen. **33** (2000) 569–578. Printed in the UK PII: S0305-4470(00)08598-X

Variational analysis for a generalized spiked harmonic oscillator

Richard L Hall† and Nasser Saad‡

† Department of Mathematics and Statistics, Concordia University, 1455 de Maisonneuve Boulevard West, Montréal, Québec, Canada H3G 1M8
‡ Department of Mathematics and Statistics, Notre-Dame University (Louaize), Zouk Mesbeh, Lebanon

Received 11 October 1999

Abstract. A variational analysis is presented for the generalized spiked harmonic oscillator Hamiltonian operator $-\frac{d^2}{dx^2} + Bx^2 + \frac{A}{x^2} + \frac{\lambda}{x^\alpha}$, where α is a real positive parameter. The formalism makes use of a basis provided by exact solutions of Schrödinger's equation for the Gol'dman and Krivchenkov Hamiltonian, and the corresponding matrix elements that were previously found. For all the discrete eigenvalues the method provides bounds which improve as the dimension D of the basis set is increased. Extension to the N-dimensional case in arbitrary angular momentum subspaces is also presented. By minimizing over the free parameter A, we are able to reduce substantially the number of basis functions needed for a given accuracy.

1. Introduction

Since the fascinating work of Harrell [1] on the ground state energy of the singular Hamiltonian $H \equiv H_0 + \lambda V = -d^2/dx^2 + x^2 + \lambda/x^\alpha$, $x \in [0, \infty]$, $\alpha > 0$, known as the spiked harmonic oscillator Hamiltonian, the volume of research in this field has grown rapidly. This is not only because of the important applications of singular Hamiltonians to a wide variety of problems in chemical, nuclear and particle physics, but also because of its intrinsically interesting properties from the point view of mathematical physics [2–5]. Most of this work [6–15], however, has focused on studying the spiked harmonic oscillator Hamiltonian in one spatial dimension since the interesting Klauder phenomenon (see [2], also [3–5]) associated with H does not occur in higher dimensions. Klauder has shown that, for sufficiently singular potentials, V cannot be turned off smoothly in the Hamiltonian H to restore the free Hamiltonian H_0. Aguilera-Navarro *et al* [6] employed variational and perturbative schemes to solve the spiked harmonic oscillator problem for the ground state energy. In their variational analysis of the Hamiltonian H, Aguilera-Navarro *et al* employed the basis set of harmonic oscillator eigenfunctions normalized in the interval $[0, \infty]$, i.e. the set of Hermite functions generated by the non-singular harmonic oscillator potential x^2.

Recently, we have obtained closed-form expressions [16] for the singular-potential integrals $\langle m|x^{-\alpha}|n\rangle$ using the Gol'dman and Krivchenkov eigenfunctions [17] for the singular Hamiltonian

$$H_0 = -\frac{d^2}{dx^2} + Bx^2 + \frac{A}{x^2} \qquad B > 0 \qquad A \geqslant 0. \tag{1.1}$$

We present a variational analysis of the generalized spiked harmonic oscillator Hamiltonian

$$H \equiv H_0 + \lambda V = -\frac{d^2}{dx^2} + Bx^2 + \frac{A}{x^2} + \frac{\lambda}{x^\alpha} \tag{1.2}$$

where λ and α are positive parameters. To evaluate the matrix elements of $x^{-\alpha}$, Hall *et al* [16] used the basis set constructed with the normalized solutions of Schrödinger's equation $H_0\psi = E\psi$, i.e.

$$\psi_n(x) \equiv |n\rangle = C_n x^{\frac{1}{2}(1+\sqrt{1+4A})} e^{-\frac{1}{2}\sqrt{B}x^2} {}_1F_1(-n, 1 + \tfrac{1}{2}\sqrt{1+4A}; \sqrt{B}x^2)$$
$$C_n^2 = \frac{2B^{\frac{1}{2}+\frac{1}{4}\sqrt{1+4A}}\Gamma(n+1+\frac{1}{2}\sqrt{1+4A})}{n![\Gamma(1+\frac{1}{2}\sqrt{1+4A})]^2} \qquad n = 0, 1, 2, \ldots \tag{1.3}$$

where ${}_1F_1$ is the confluent hypergeometric function [18]

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

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

$$\langle m|x^{-\alpha}|n\rangle = (-1)^{n+m} B^{\alpha/4} \sqrt{\frac{\Gamma(\gamma+m)}{n!m!\,\Gamma(\gamma+n)}} \times \sum_{k=0}^{m} (-1)^k \binom{m}{k} \frac{\Gamma(k+\gamma-\frac{\alpha}{2})\Gamma(\frac{\alpha}{2}-k+n)}{\Gamma(k+\gamma)\Gamma(\frac{\alpha}{2}-k)} \tag{1.4}$$
$$\gamma = 1 + \frac{1}{2}\sqrt{1+4A}$$

in which each element has a factor which is a polynomial of degree $m + n$ in α. Of particular interest are the matrix elements $\langle 0|x^{-\alpha}|n\rangle$, which can be obtained from equation (1.4), and read as follows:

$$\langle 0|x^{-\alpha}|n\rangle = (-1)^n B^{\alpha/4} \sqrt{\frac{\Gamma(\gamma)}{n!\,\Gamma(\gamma+n)}} \frac{\Gamma(\gamma-\frac{\alpha}{2})\Gamma(\frac{\alpha}{2}+n)}{\Gamma(\gamma)\Gamma(\frac{\alpha}{2})} \qquad n = 0, 1, 2, \ldots. \tag{1.5}$$

The special case where $A = 0$ and $B = 1$ allows us to recover the matrix elements provided by Aguilera-Navarro *et al* [6] for the operator $x^{-\alpha}$ in the harmonic oscillator representation, supplemented by the Dirichlet boundary condition $\psi(0) = 0$. Indeed, substituting $A = 0$ and $B = 1$, and using the identities

$$\frac{\Gamma(n+\frac{3}{2})}{\Gamma(\frac{3}{2})} = \frac{(2n+1)!}{2^{2n}n!} \qquad \frac{\Gamma(z+n)}{\Gamma(z)} = (z+n-1)(z+n-2)\ldots(z+1)z$$

after some algebraic simplification, we can easily show that equation (1.4) reduces to equation (12) and equation (13), for $m = 0$, of [6]. All these expressions are valid for $\alpha < 3$.

The purpose of this paper is to employ the variational method, with the matrix elements (1.4), to solve the generalized singular Schrödinger equation

$$\left[-\frac{d^2}{dx^2} + Bx^2 + \frac{A}{x^2} + \frac{\lambda}{x^\alpha}\right]\psi = E\psi \qquad 0 \leqslant x < \infty. \tag{1.6}$$

This paper is a generalization of the variational approach of Aguilera-Navarro *et al* [6] that used harmonic oscillator functions and was restricted to the ground state level ($B = 1$, $A = 0$).

The paper is organized as follows. In section 2, we outline the variational method used to study (1.6), and we also extend the scope to cover the N-dimensional case. Some numerical results, and comparisons with the results of Aguilera-Navarro *et al*, are presented in section 3. In section 4 it is shown that a further optimization over the free parameter A reduces substantially the number of basis functions needed to compute the eigenvalues to a given accuracy.

2. The variational method

The first step in the variational method is to select a suitable complete set of basis functions that is adapted to the problem at hand. In the variational analysis of the ground state energy of the singular potential $V(x) = x^2 + \lambda x^{-\alpha}$, known in the literature as the spiked harmonic oscillator potential, Aguilera-Navarro *et al* employed a basis set of harmonic oscillator eigenfunctions normalized on the interval $[0, \infty]$ and vanishing at $x = 0$, i.e. the set of odd Hermite functions generated by the non-singular harmonic oscillator potential x^2. A more effective basis set for the variational analysis of such singular problems is the set of normalized wavefunctions (1.3) because the singular characteristics of the potential are naturally built into the wavefunctions.

Let $\psi(x)$ be a 'trial function' for Hamiltonian H given by (1.2), and let us suppose that $\psi(x)$ can be expanded in terms of the basis set $\psi_n(x)$ defined by (1.3). Thus we have

$$\psi(x) = \sum_{n=0}^{D-1} a_n \psi_n(x). \tag{2.1}$$

The problem now is to minimize the eigenenergies of (1.2) with respect to the variational parameters a_n, $n = 0, 1, \ldots, D-1$, in the finite-dimensional subspace H_D spanned by the D functions $\psi_0, \psi_1, \ldots, \psi_{D-1}$. This variational problem is equivalent to diagonalizing the Hamiltonian (1.2) in the subspace H_D. By increasing the dimension D, we can always improve the results. Thus, we have to evaluate the matrix elements of the Hamiltonian (1.2) in the basis (1.3). They can be separated into two contributions

$$H_{mn} = \langle m|H|n\rangle \equiv \langle m|H_0|n\rangle + \lambda\langle m|x^{-\alpha}|n\rangle \qquad m, n = 0, 1, 2, \ldots, D-1. \tag{2.2}$$

Since H_0 is diagonal in the chosen basis, the first term on the right-hand side of (2.2) is the exact solution of the Gol'dman and Krivchenkov Hamiltonian, that is

$$\langle m|H_0|n\rangle = \sqrt{B}(4n + 2 + \sqrt{1+4A})\delta_{mn} \qquad m, n = 0, 1, 2, \ldots, D-1 \tag{2.3}$$

where δ_{mn} is the Kronecker delta that equals 1 if $m = n$ and 0 if $m \neq m$. The second term is given by the matrix elements (1.4). Explicit expressions for the first 15 matrix elements of $x^{-\alpha}$ are given in the appendix.

In order to extend the scope of this analysis to the N-dimensional Schrödinger equation (1.8), we observe first that the A term has the dimensions of kinetic energy, such as the term that appears in higher-dimensional systems. We may therefore replace A in equation (2.2) with

$$A \rightarrow A + (l + \tfrac{1}{2}(N-1))(l + \tfrac{1}{2}(N-3)) \qquad N \geqslant 2 \tag{2.4}$$

where the unperturbed energy levels (2.3) become in this case

$$\langle m|H_0|n\rangle = 2\sqrt{B}\left(2n + 1 + \sqrt{A + \left(l + \frac{N}{2} - 1\right)^2}\right)\delta_{mn} \qquad N \geqslant 2. \tag{2.5}$$

Thus, equation (2.2) becomes

$$H_{mn} = 2\sqrt{B}\left(2n + 1 + \sqrt{A + \left(l + \frac{N}{2} - 1\right)^2}\right)\delta_{mn} + \lambda\langle m|x^{-\alpha}|n\rangle$$
$$m, n = 0, 1, 2, \ldots, D-1 \tag{2.6}$$

where the matrix elements $\langle m|x^{-\alpha}|n\rangle$ become

$$\langle m|x^{-\alpha}|n\rangle = (-1)^{n+m} B^{\frac{\alpha}{4}} \sqrt{\frac{\Gamma(m + 1 + \sqrt{A + (l + N/2 - 1)^2})}{n!m!\,\Gamma(n + 1 + \sqrt{A + (l + N/2 - 1)^2})}}$$

$$\times \sum_{k=0}^{m}(-1)^k\binom{m}{k}\frac{\Gamma(k-\frac{\alpha}{2}+1+\sqrt{A+(l+N/2-1)^2})\Gamma(\frac{\alpha}{2}-k+n)}{\Gamma(k+l+\sqrt{A+(l+N/2-1)^2})\Gamma(\frac{\alpha}{2}-k)}$$
$$N \geqslant 2. \qquad (2.7)$$

We have omitted the case $N = 1$ because this curious singular problem in one dimension has features [19–21] that are not in harmony with our main purpose.

To recover the results of Aguilera-Navarro *et al*, we substitute $A = 0$, $B = 1$, $N = 3$, and $l = 0$ in equation (2.6). In other words, we obtain a general variational expression (2.2) that treats the solution of Schrödinger's equations (1.8), and also the work of Aguilera-Navarro *et al* in a single formulation.

3. Some numerical results

From equations (2.2), (2.3), and (1.4) and the results given in the appendix it can be readily seen that the first variational approximation (subspace of dimension one) to the ground state eigenvalues of the Hamiltonian (1.2) is

$$E_0 = H_{00} = \langle 0|H|0\rangle = 2\sqrt{B}\gamma + \lambda B^{\frac{\alpha}{4}}\frac{\Gamma(\gamma-\frac{\alpha}{2})}{\Gamma(\gamma)} \qquad \gamma = 1+\frac{1}{2}\sqrt{1+4A}. \qquad (3.1)$$

For the case $A = 0$ and $B = 1$, E_0 reduces to

$$E^{(0)} = 3 + \lambda\frac{\Gamma(\frac{3-\alpha}{2})}{\Gamma(\frac{3}{2})} \qquad (3.2)$$

which coincides with the ground state energy expression for the spiked harmonic oscillator obtained by Aguilera-Navarro *et al*, i.e. equation (5.1) in [6].

When $D = 2$ the diagonalization can also be performed analytically, by means of the secular equation, and we obtain

$$E_{\pm} = \frac{1}{2}\Bigg[4\sqrt{B}(1+\gamma) + \frac{\lambda}{4}B^{\frac{\alpha}{4}}(\alpha^2-2\alpha+8\gamma)\frac{\Gamma(\gamma-\frac{\alpha}{2})}{\Gamma(\gamma+1)}$$
$$\pm\sqrt{16B + 2\lambda B^{\frac{\alpha+2}{4}}\alpha(\alpha-2)\frac{\Gamma(\gamma-\frac{\alpha}{2})}{\Gamma(\gamma+1)} + \frac{\lambda^2}{16}B^{\frac{\alpha}{2}}\alpha^2((\alpha-2)^2+16\gamma)\left[\frac{\Gamma(\gamma-\frac{\alpha}{2})}{\Gamma(\gamma+1)}\right]^2}\,\Bigg] \qquad (3.3)$$

where $E_0 = E_-$ and $E_1 = E_+$. Again, if we put $A = 0$, $B = 1$, and $\alpha = \frac{5}{2}$ we obtain

$$E_{\pm} = \frac{1}{2}\left[10 + \frac{53}{24}\lambda\frac{\Gamma(\frac{3-\alpha}{2})}{\Gamma(\frac{3}{2})} \pm \sqrt{16 + \frac{5}{2}\lambda\frac{\Gamma(\frac{3-\alpha}{2})}{\Gamma(\frac{3}{2})} + \frac{2425}{576}\lambda^2\left[\frac{\Gamma(\frac{3-\alpha}{2})}{\Gamma(\frac{3}{2})}\right]^2}\,\right] \qquad (3.4)$$

which coincides with equation (5.2) in [6].

For higher values of the variational space dimension D we have to use a numerical diagonalization procedure such as that of Jacobi [22] to find the eigenvalues of the matrix $\mathcal{H}$ given by

$$\mathcal{H} = \begin{pmatrix} H_{00} & H_{01} & \dots & H_{0D-1} \\ H_{10} & H_{11} & \dots & H_{1D-1} \\ \dots & \dots & \dots & \dots \\ H_{D-10} & H_{D-11} & \dots & H_{D-1D-1} \end{pmatrix}. \qquad (3.5)$$

Table 1 shows the convergence of these results, when $\alpha = 2.5$, for the ground state energy (i.e. $A = 0$, $B = 1$) of the spiked harmonic oscillator, and selected values of λ. For this special

Table 1. The ground state eigenvalue of Schrödinger's equation $H\psi = E\psi$, where $A = 0$ and $H = -\frac{d^2}{dx^2} + x^2 + \frac{\lambda}{x^{2.5}}$ is obtained by diagonalization of the $D \times D$ matrix elements with $D = 1, 2, 10, 20, 30$. The 'exact' values E were obtained by direct numerical integration of Schrödinger's equation.

λ	$E^{(1)}$	$E^{(2)}$	$E^{(10)}$	$E^{(20)}$	$E^{(30)}$	E
1000	4094.062 692	324.897 482	44.967 048	44.955 485	44.955 485	44.955 485
100	412.106 269	36.802 319	17.541 891	17.541 890	17.541 890	17.541 890
10	43.910 627	7.951 034	7.735 637	7.735 135	7.735 114	7.735 111
5	23.455 313	6.304 224	6.297 319	6.296 710	6.296 566	6.296 473
1	7.091 063	4.688 098	4.354 248	4.329 430	4.323 263	4.317 312
0.5	5.045 531	4.216 200	3.919 692	3.882 149	3.869 547	3.848 553
0.1	3.409 106	3.366 867	3.316 061	3.302 484	3.296 024	3.266 871
0.05	3.204 553	3.193 800	3.177 840	3.172 753	3.170 127	3.152 420
0.01	3.040 911	3.040 476	3.039 702	3.039 409	3.039 244	3.036 665
0.005	3.020 455	3.020 346	3.020 148	3.020 071	3.020 027	3.019 086
0.001	3.004 091	3.004 087	3.004 079	3.004 075	3.004 074	3.004 014

Table 2. Upper bounds E_{00}^N for $A = 0$ and $H = -\frac{d^2}{dx^2} + x^2 + \frac{10}{x^{1.9}}$ for dimension $N = 2$–10, obtained by diagonalization of the $D \times D$ matrix $\mathcal{H}$, $D = 1, 2, 10, 20, 30$. The 'exact' values E were obtained by direct numerical integration of Schrödinger's equation.

N	$E^{(1)}$	$E^{(2)}$	$E^{(10)}$	$E^{(20)}$	$E^{(30)}$	E
2	196.700 853	9.092 284	8.485 580	8.485 399	8.485 384	8.485 378
3	21.236 010	8.698 978	8.564 442	8.564 364	8.564 358	8.564 356
4	13.735 043	8.813 825	8.795 449	8.795 440	8.795 440	8.795 440
5	11.686 537	9.163 174	9.163 095	9.163 094	9.163 093	9.163 093
6	11.110 897	9.650 211	9.646 713	9.646 702	9.646 701	9.646 701
7	11.145 653	10.233 096	10.225 061	10.225 046	10.225 045	10.225 045
8	11.492 447	10.889 178	10.879 092	10.879 078	10.879 077	10.879 077
9	12.020 404	11.603 187	11.592 993	11.592 982	11.592 982	11.592 982
10	12.662 990	12.363 513	12.354 191	12.354 183	12.354 183	12.354 183

case with $A = 0$ and $\alpha = \frac{5}{2}$, our results confirm those of [6] (*their* table I), except for minor rounding errors: it appears that the results of Aguilera-Navarro *et al* have been truncated rather than rounded. It is important to mention here that, although the matrix element $x_{33}^{-\alpha}$, reported in [6], contains some errors in the coefficients for the exponent α, the results in table I of [6] are correct. Indeed, $x_{33}^{-\alpha}$ should read

$$x_{33}^{-\alpha} = \frac{\Gamma\left(\frac{3-\alpha}{2}\right)}{7!\Gamma\left(\frac{3}{2}\right)}(\alpha^6 - 6\alpha^5 + 106\alpha^4 - 384\alpha^3 + 2080\alpha^2 - 3408\alpha + 5040) \tag{3.6}$$

instead of

$$x_{33}^{-\alpha} = \frac{\Gamma\left(\frac{3-\alpha}{2}\right)}{7!\Gamma\left(\frac{3}{2}\right)}(\alpha^6 - 6\alpha^5 + 106\alpha^4 - 454\alpha^3 + 1660\alpha^2 - 3968\alpha + 5040) \tag{3.7}$$

as quoted by Aguilera-Navarro *et al* [6]. The results quoted in their table I must therefore have been calculated with the correct formula. We have also corrected in the appendix here some errors in the coeffecients of the general matrix element $x_{33}^{-\alpha}$ presented in [16].

In table 2 we report the upper bounds $E_{nl} = E_{00}^N$ obtained for the Hamiltonian $H = -\frac{d^2}{dx^2} + x^2 + \frac{10}{x^{1.9}}$ in spatial dimensions $N = 2$–10. Now the value of A depends on the angular momentum ℓ and the number of spatial dimension N as determined by equation (2.4).

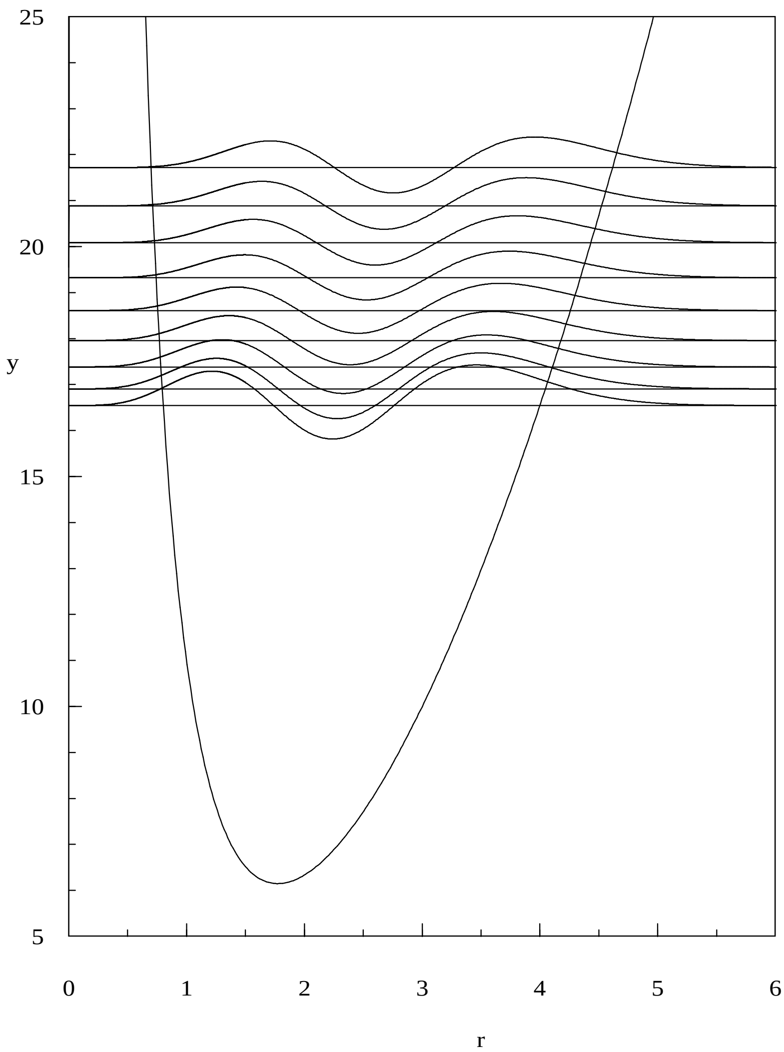

Figure 1. The potential $y = V(r)$, and the nine wavefunctions corresponding to the eigenvalues $E_{n\ell} = E_{21}$ for spatial dimensions $N = 2$–10.

As we mentioned above, the method we discussed in section 2 provides bounds on *all* the eigenvalues in a given angular momentum subspace. We present in table 3 our results for the eigenvalues $E_{nl} = E_{21}^{N}$ for spatial dimensions $N = 2$–10; the potential and the corresponding wavefunctions are shown in figure 1. For comparison, we have integrated Schrödinger's equation numerically, with the Hamiltonian given by (1.2), for different values of exponent α. To avoid difficulties caused by the singular character of the potential near the origin, we begin the integrations near the potential minimum and integrate in both directions, away from the starting point. A similar approach has been described by Diaz *et al* [23].

Table 3. Upper bounds E_{21}^N for $A = 0$ and $H = -\Delta + x^2 + \frac{10}{x^{2.1}}$ for dimensions $N = 2$–10, obtained by diagonalization of the $D \times D$ matrix $\mathcal{H}$ for $D = 30$. The 'exact' values E_{21} were obtained by direct numerical integration of Schrödinger's equation.

N	E_{21}^N	E_{21}
2	16.543 648	16.543 629
3	16.904 446	16.904 445
4	17.381 709	17.381 708
5	17.955 446	17.955 444
6	18.607 070	18.607 067
7	19.320 693	19.320 691
8	20.083 407	20.083 406
9	20.885 022	20.885 021
10	21.717 608	21.717 608

Table 4. Eigenvalues of Schrödinger's equation $H\psi = E\psi$, where $H = -\frac{d^2}{dx^2} + x^2 + \frac{\lambda}{x^{2.5}}$ obtained by diagonalization of the $n \times n$ matrix $\mathcal{H}$, $n = 1, 2, \ldots, 5$ and minimizing over the parameter A.

λ	$E^{(1)}$	$E^{(2)}$	$E^{(3)}$	$E^{(4)}$	$E^{(5)}$	E
1000	44.959 423	44.955 722	44.955 562	44.955 559	44.955 517	44.955 485
100	17.546 305	17.542 630	17.542 082	17.542 066	17.542 040	17.541 890
10	7.408 73	7.736 864	7.735 869	7.735 645	7.735 596	7.735 111
5	6.302 942	6.298 821	6.297 638	6.297 281	6.297 145	6.296 473
1	3.325 682	4.321 615	4.320 076	4.319 376	4.318 963	4.317 312
0.5	3.857 330	3.853 611	3.852 085	3.851 313	3.850 823	3.848 553
0.1	3.273 542	3.271 566	3.270 632	3.270 082	3.269 700	3.266 871
0.05	3.157 126	3.155 956	3.155 378	3.155 022	3.154 768	3.152 420
0.01	3.037 845	3.037 674	3.037 581	3.037 520	3.037 474	3.036 665
0.005	3.019 610	3.019 553	3.019 522	3.019 500	3.019 484	3.019 086
0.001	3.004 053	3.004 050	3.004 049	3.004 048	3.004 047	3.004 014

4. A further variational refinement

We now introduce another variational adjustment that will substantially reduce the number of basis elements required to compute the eigenvalues of the Hamiltonian, i.e.

$$H = -\frac{d^2}{dx^2} + \frac{(l + \frac{1}{2}(N-1))(l + \frac{1}{2}(N-3))}{x^2} + Bx^2 + \frac{\lambda}{x^\alpha}. \tag{4.1}$$

We notice first that the Hamiltonian (4.1) can be written as

$$H = -\frac{d^2}{dx^2} + \frac{(l + \frac{1}{2}(N-1))(l + \frac{1}{2}(N-3))}{x^2} + Bx^2 + \frac{A}{x^2} + \left(\frac{\lambda}{x^\alpha} - \frac{A}{x^2}\right) \tag{4.2}$$

where A is an additional variational parameter, different from zero, to be determined later. In this case equation (2.2) becomes

$$H_{mn} = 2\sqrt{B}(2n + 1 + \sqrt{A + (l + N/2 - 1)^2})\delta_{mn} + \lambda\langle m|x^{-\alpha}|n\rangle - A\langle m|x^{-2}|n\rangle \tag{4.3}$$

where $\langle m|x^{-\alpha}|n\rangle$ is given by (2.7) and $\langle m|x^{-2}|n\rangle$ is obtained by setting $\alpha = 2$ in this formula. Upper bounds to the eigenvalues E_{nl}^N are again provided by finding the eigenvalues of the matrix $\mathcal{H}$ given by equation (3.5), but with the entries depending on A according to (4.3).

For example, when the variational space has dimension $D = 1$, the lowest eigenvalue of the problem in N dimensions labelled by l is determined by

$$H_{00} = \sqrt{B}(2\gamma - \frac{A}{\gamma - 1}) + \lambda B^{\alpha/4}\frac{\Gamma(\gamma - \frac{\alpha}{2})}{\Gamma(\gamma)} \tag{4.4}$$

where $\gamma = 1 + \sqrt{A + (l + \frac{N}{2} - 1)^2}$. For $N = 3, l = 0$, the minimum of H_{00} with respect to A for $\alpha = 2$ occurs at $A = \lambda$, thus yielding the exact solution of the spiked harmonic oscillator $E_0 = \sqrt{B}(1 + \sqrt{1 + 4A})$. In fact, a 'good' general estimate for the value of A is $A = \lambda$. This rough estimate for A reduces substantially the number of the basis function needed to compute the eigenvalues; by minimizing over A, we obtain even better upper bounds, as table 4 clearly indicates.

5. Conclusion

We have generalized the work of Aguilera-Navarro *et al* to treat the more general spiked harmonic oscillator problem (1.2). In particular, we have presented a variation method to solve the interesting N-dimensional spiked harmonic oscillator problem with the $x^{-\alpha}$ singular term. The present work is limited by the necessary condition $\alpha < 3$. Some interesting results for $\alpha \geqslant 3$ may be found, for example, in [24–26].

We hope that our work will encourage further research into the spectra generated by this interesting class of singular potentials. It is very clear from our results that use of a variational basis which is itself derived from a related soluble singular problem leads to very effective approximation methods for more general problems of this singular type. The presence of the free parameter A in the class of soluble problems allows a further refinement in the upper energy estimates.

Acknowledgment

Partial financial support of this work under Grant No GP3438 from the Natural Sciences and Engineering Research Council of Canada is gratefully acknowledged by one of us (RLH).

Appendix. Some explicit forms of the matrix elements $\langle m|x^{-\alpha}|n\rangle$

We present the first 15 matrix elements of $x^{-\alpha}$ that we used to compute the variational eigenvalues in this paper. Some errors in the coefficients of $x_{33}^{-\alpha}$ in [16] have been corrected. In terms of the parameter $\gamma = 1 + \frac{1}{2}\sqrt{1 + 4A}$, the explicit matrix elements, from equation (1.4) and equation (1.5), are as follows:

$$x_{nm}^{-\alpha} \equiv \langle m|x^{-\alpha}|n\rangle$$

$$x_{00}^{-\alpha} = B^{\frac{\alpha}{4}} \frac{\Gamma(-\frac{\alpha}{2} + \gamma)}{\Gamma(\gamma)}$$

$$x_{01}^{-\alpha} = -B^{\frac{\alpha}{4}} \frac{\alpha}{2\sqrt{\gamma}} \frac{\Gamma(-\frac{\alpha}{2} + \gamma)}{\Gamma(\gamma)}$$

$$x_{02}^{-\alpha} = B^{\frac{\alpha}{4}} \frac{\alpha(\alpha + 2)}{2^2\sqrt{2!\gamma(\gamma + 1)}} \frac{\Gamma(-\frac{\alpha}{2} + \gamma)}{\Gamma(\gamma)}$$

$$x_{03}^{-\alpha} = -B^{\frac{\alpha}{4}} \frac{\alpha(\alpha + 2)(\alpha + 4)}{2^3\sqrt{3!\gamma(\gamma + 1)(\gamma + 2)}} \frac{\Gamma(-\frac{\alpha}{2} + \gamma)}{\Gamma(\gamma)}$$

$$x_{04}^{-\alpha} = B^{\frac{\alpha}{4}} \frac{\alpha(\alpha + 2)(\alpha + 4)(\alpha + 6)}{2^4\sqrt{4!\gamma(\gamma + 1)(\gamma + 2)(\gamma + 3)}} \frac{\Gamma(-\frac{\alpha}{2} + \gamma)}{\Gamma(\gamma)}$$

$$x_{11}^{-\alpha} = B^{\frac{\alpha}{4}} \frac{(\alpha^2 - 2\alpha + 4\gamma)}{2^2} \frac{\Gamma(-\frac{\alpha}{2} + \gamma)}{\Gamma(\gamma + 1)}$$

$$x_{12}^{-\alpha} = -B^{\frac{\alpha}{4}} \frac{\alpha(\alpha^2 - 2\alpha + 8\gamma)}{2^3\sqrt{2!(\gamma+1)}} \frac{\Gamma(-\frac{\alpha}{2}+\gamma)}{\Gamma(\gamma+1)}$$

$$x_{13}^{-\alpha} = B^{\frac{\alpha}{4}} \frac{\alpha(\alpha+2)(\alpha^2 - 2\alpha + 12\gamma)}{2^4\sqrt{3!(\gamma+1)(\gamma+2)}} \frac{\Gamma(-\frac{\alpha}{2}+\gamma)}{\Gamma(\gamma+1)}$$

$$x_{14}^{-\alpha} = -B^{\frac{\alpha}{4}} \frac{\alpha(\alpha+2)(\alpha+4)(\alpha^2 - 2\alpha + 16\gamma)}{2^5\sqrt{4!(\gamma+1)(\gamma+2)(\gamma+3)}} \frac{\Gamma(-\frac{\alpha}{2}+\gamma)}{\Gamma(\gamma+1)}$$

$$x_{22}^{-\alpha} = B^{\frac{\alpha}{4}} \frac{\alpha^4 - 4\alpha^3 + (12+16\gamma)\alpha^2 - (16+32\gamma)\alpha + 32\gamma(1+\gamma)}{2^4\sqrt{2!2!}} \frac{\Gamma(-\frac{\alpha}{2}+\gamma)}{\Gamma(\gamma+2)}$$

$$x_{23}^{-\alpha} = -B^{\frac{\alpha}{4}} \frac{\alpha(\alpha^4 - 4\alpha^3 + (20+24\gamma)\alpha^2 - (32+48\gamma)\alpha + 96\gamma(1+\gamma))}{2^5\sqrt{2!3!(\gamma+2)}} \frac{\Gamma(-\frac{\alpha}{2}+\gamma)}{\Gamma(\gamma+2)}$$

$$x_{24}^{-\alpha} = B^{\frac{\alpha}{4}} \frac{\alpha(\alpha^5 - 2\alpha^4 + (20+32\gamma)\alpha^3 + 8\alpha^2 + (-96+64\gamma+192\gamma^2)\alpha + 384\gamma(\gamma+1))}{2^6\sqrt{2!4!(\gamma+2)(\gamma+3)}} \times \frac{\Gamma(-\frac{\alpha}{2}+\gamma)}{\Gamma(\gamma+2)}$$

$$x_{33}^{-\alpha} = \frac{B^{\frac{\alpha}{4}}}{2^6\sqrt{3!3!}}(\alpha^6 - 6\alpha^5 + (52+36\gamma)\alpha^4 - (168+144\gamma)\alpha^3 + (352+720\gamma+288\gamma^2)\alpha^2 - (384+1152\gamma+576\gamma^2)\alpha + 384\gamma(1+\gamma)(2+\gamma)) \frac{\Gamma(-\frac{\alpha}{2}+\gamma)}{\Gamma(\gamma+3)}$$

$$x_{34}^{-\alpha} = -\frac{B^{\frac{\alpha}{4}}}{2^7\sqrt{3!4!(\gamma+3)}}(\alpha^7 - 6\alpha^6 + (76+48\gamma)\alpha^5 - (264+192\gamma)\alpha^4 + (832+1536\gamma+576\gamma^2)\alpha^3 - (1152+2688\gamma+1152\gamma^2)\alpha^2 + 1536\gamma(\gamma+1)(\gamma+2)\alpha) \frac{\Gamma(-\frac{\alpha}{2}+\gamma)}{\Gamma(\gamma+3)}$$

$$x_{44}^{-\alpha} = \frac{B^{\frac{\alpha}{4}}}{2^8\sqrt{4!4!}}(\alpha^8 - 8\alpha^7 + (136+64\gamma)\alpha^6 - (704+384\gamma)\alpha^5 + (3856+4480\gamma+1152\gamma^2)\alpha^4 - (10\,880+15\,360\gamma+4608\gamma^2)\alpha^3 + (19\,200+48\,640\gamma+32\,256\gamma^2+6144\gamma^3)\alpha^2 - (18\,432+67\,584\gamma+55\,296\gamma^2+12\,288\gamma^3)\alpha + 6144\gamma(\gamma+1)(\gamma+2)(\gamma+3)) \frac{\Gamma(-\frac{\alpha}{2}+\gamma)}{\Gamma(\gamma+4)}.$$

References

[1] Harrell E M 1977 *Ann. Phys.* **105** 379
[2] Klauder J R 1973 *Acta Phys. Austriaca Suppl.* **11** 341
[3] Detwiler L C and Klauder J R 1975 *Phys. Rev.* D **11** 1436
[4] Simon B 1973 *J. Funct. Anal.* **14** 295
[5] DeFacio B and Hammer C L 1974 *J. Math. Phys.* **15** 1071
[6] Aguilera-Navarro V C, Estévez G A and Guardiola R 1990 *J. Math. Phys.* **31** 99
[7] Aguilera-Navarro V C and Guardiola R 1991 *J. Math. Phys.* **32** 2135
[8] Solano-Torres, Estéves G A, Fernández F M and Groenenboom G C 1992 *J. Phys. A: Math. Gen.* **25** 3427
[9] Flynn M F, Guardiola R and Znojil M 1993 *Czech. J. Phys.* **41** 1019
[10] Znojil M 1992 Proc. Int. Conf. on Hadron Structure ’91 *Proc. CSFR* vol 1, p 1
[11] Znojil M 1993 *J. Math. Phys.* **34** 4914

[12] Estévez-Bretón E S and Estévez-Bretón G A 1993 *J. Math. Phys.* **34** 437

[13] Hall R and Saad N 1995 *Can. J. Phys.* **73** 493

[14] Hall R and Saad N 1998 *J. Phys. A: Math. Gen.* **31** 963

[15] Hall R and Saad N 1999 *J. Phys. A: Math. Gen.* **32** 133

[16] Hall R, Saad N and von Keviczky A 1998 *J. Math. Phys.* **39** 6345–51

[17] Gol'dman I I and Krivchenkov D V 1961 *Problems in Quantum Mechanics* (London: Pergamon)

[18] Slater L J 1960 *Confluent Hypergeometric Functions* (Cambridge: Cambridge University Press)

[19] Bhattacharyya K and Pathak R K 1996 *Int. J. Quantum Chem.* **59** 219–26

[20] Ballhausen C J 1988 *Chem. Phys. Lett.* **146** 449

[21] Senn P 1989 *Chem. Phys. Lett.* **154** 172

[22] Press H W, Flannery P B, Teukolsky A S and Vetterling T W 1989 *Numerical Recipes in Pascal: The Art of Scientific Computing* (Cambridge: Cambridge University Press)

[23] Diaz C G, Fernández F M and Castro E A 1988 *J. Phys. A: Math. Gen.* **21** L11

[24] Papp E 1989 *Europhys. Lett.* **9** 309

[25] Znojil M 1999 *Phys. Lett.* A **255** 1

[26] Znojil M 1999 *Phys. Lett.* A **259** 220