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On the eigenvalues of the s-state radial equation of a spiked harmonic oscillator

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Abstract. Eigenvalues of the ground state of the radial Schrödinger equation for a spiked harmonic-oscillator potential have been evaluated employing two methods: numerically, via the Lanczos/grid technique, and by means of standard Padé approximants constructed from an expansion of large coupling parameter series for the energy. Numerical results are compared for several values of the parameters characterizing the spiked singular potential.

1. Introduction

The solution of the one-particle Schrödinger equation employing singular perturbation potentials has been a subject of continuous interest during the past two decades. Analytical as well as numerical solutions have been attempted. Among the former, the seminal work by Case (1950), and the stimulating articles by Spector (1965, 1967), Klauder (1973, 1975, 1978), Detwiler and Klauder (1975), Ezawa *et al* (1975), Harrel (1977), Znojil (1982, 1984, 1989, 1990, 1991a, b) and Flynn *et al* (1991) are worth mentioning. Many innovative and simple methods for numerically integrating the Schrödinger equation have been developed. Of special relevance to this article are the works by Killingbeck (1977, 1979, 1980a, b, 1982, 1985, 1988), Hajj (1980), Korsch and Laurent (1981), Giraldo *et al* (1985, 1986), García and Caro (1987) and Groenenboom and Buck (1990). Further references on the numerical and analytical solution of the non-relativistic Schrödinger equation can be found in the works cited above. Quite recently, Aguilera-Navarro *et al* (1990) have outlined simple seminumerical techniques to find the ground state energy of a spiked harmonic-oscillator Hamiltonian. The principal thrust of the latter article was a large coupling perturbative expansion analysis for the energy. Such treatment presents great challenges since an extremely high order of accuracy in the calculations must be observed if meaningful and reliable results are to be obtained from these calculations. Killingbeck (1982) has pointed out that Detwiler and Klauder (1975) reported results for the eigenenergies

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of the spiked harmonic-oscillator Hamiltonian that were vitiated because of the program employed by these workers to compute the eigenvalues in question. The twofold purpose of this short article is:

(i) to present independent checks to the results reported by Killingbeck (1982) and thus resolve conclusively the issue of the discrepancy between the eigenenergy values given by this author and those of Detwiler and Klauder (1975); and

(ii) to propose an accurate, analytical approximation for the ground state energy of the spiked harmonic oscillator, applicable to arbitrary values of the strength parameter.

2. Background

As has been pointed out by Harrel (1977), de Llano (1981), Znojil (1982, 1984, 1989, 1990) and others, there are a number of cases where the use of singular potentials is of interest physically and mathematically. The particular type of singular perturbation potential to be treated in this paper is $\lambda r^{-\alpha}$, where r is the radial coordinate. Throughout this article the adjective 'spiked' will be employed to denote an $r^{-\alpha}$ term in the potential. A true spike (a Dirac delta) has been employed by Killingbeck (1988) to find $\psi^2(x)$ as an expectation value. As is well known, the $\lambda r^{-\alpha}$ term characterizes a repulsive core interaction in quantum mechanics and its effect becomes negligibly small away from $r=0$. The quantity λ (>0) measures the strength of the perturbative potential term. The higher the value of the positive parameter α, the stronger the singularity of the perturbation potential at the origin. The s-state radial equation of a spiked harmonic oscillator reads

$$-D^2\Psi + r^2\Psi + \lambda r^{-\alpha}\Psi = E\Psi \tag{1}$$

with the Dirichlet boundary condition $\Psi(0)=0$, where $\Psi(r)$ denotes a real-valued solution of the time-independent Schrödinger equation. The interval of interest for the radial distance is $(0, \infty)$.

3. Methods of calculation

A method to calculate the ground state energy of the spiked harmonic oscillator has been described in an interesting and important paper by Detwiler and Klauder (1975). In an attempt to check the relative merits of the sets of results derived by Detwiler and Klauder (1975) and those found by Killingbeck (1982), we have numerically solved the Schrödinger equation for the spiked harmonic oscillator for several values of α and λ. For this task we have employed the Lanczos/grid method developed and successfully tested by Groenenboom and Buck (1990). Essentially the method consists in discretizing the Hamiltonian $-D^2+r^2+\lambda r^{-\alpha}$ on a grid. In the present work $r_{\min} \ldots r_{\max} = 0.0 \ldots 6.0$. Six different values for the number N of grid points were employed, namely 100, 200, 400, 800, 1600 and 3200. The h values are $6/N$. A tenth-order finite difference formula was employed for the kinetic energy. The Lanczos iteration (Lanczos 1950, Cullum and Willoughby 1981) was started with the function $r^8 \exp(-r^2)$. Table 1 shows the ground state energy eigenvalues E_i corresponding to the six different N values in the finite difference representation of the Hamiltonian (1). For the sake

Table 1. The energies for six different N values in the finite difference representation of the Hamiltonian given by equation (1). The error estimate error_1 for E_i is simply $E_i - E_{i+1}$. *Error_2 is the bisection routine error estimate.* The underlined values are the most accurate ones.

		$\alpha = 4$			$\alpha = 6$		
λ	N	Energy	Error_1	Error_2	Energy	Error_1	Error_2
0.01	100	3.205 248 45	−2.1E−04	2.0E−12	3.505 321 54	1.3E−04	2.0E−10
	200	3.205 035 67	3.2E−05	1.6E−11	3.505 452 15	2.4E−07	1.3E−08
	400	3.205 067 73	−2.5E−07	2.1E−10	3.505 452 39	1.8E−06	8.4E−07
	800	3.205 067 48	1.6E−08	3.2E−09	3.505 454 14		5.3E−05
	1600	3.205 067 49	−8.1E−09	5.0E−08			
	3200	3.205 067 49		8.1E−07			
0.005	100	3.144 946 96	3.7E−03	1.9E−12	3.422 915 17	−3.3E−05	1.0E−10
	200	3.148 597 05	−2.6E−04	1.0E−11	3.422 881 89	2.3E−06	6.5E−09
	400	3.148 333 77	1.8E−05	1.2E−10	3.422 884 16	3.1E−06	4.2E−07
	800	3.148 352 23	7.4E−08	1.6E−09	3.422 887 27		2.7E−05
	1600	3.148 352 31	−1.2E−09	2.5E−08			
	3200	3.148 352 31		4.0E−07			
0.0025	100	3.097 740 34	9.2E−03	1.9E−12	3.354 181 54	−2.6E−04	5.2E−11
	200	3.106 894 92	−1.0E−04	8.0E−12	3.353 918 86	4.4E−07	3.2E−09
	400	3.106 793 92	1.5E−05	6.6E−11	3.353 919 30	4.7E−07	2.1E−07
	800	3.106 809 05	−1.2E−07	8.6E−10	3.353 919 77		1.3E−05
	1600	3.106 808 93	1.3E−08	1.3E−08			
	3200	3.106 808 95		2.0E−07			

of completeness, a simple error, estimate $\text{error}_1 = E_i - E_{i+1}$ for the energies E_i has also been included in the table. From table 1 it is inferred that only a limited accuracy of the results can be obtained, particularly for the case for which $\alpha = 6$. This is to be expected because, as has been remarked earlier, when the parameter α is relatively large the spikelike term in the potential energy function becomes more singular at the origin. The program employed in the present work to determine the eigenvalues of the spiked harmonic oscillator makes use of the bisection algorithm (Wilkinson and Reinsch 1971). This routine gives an error bound estimate, error_2 in table 1, which is related to the norm of the matrix. Figure 1 shows plots of this bisection-error estimate, together with the error estimate $E_i - E_{i+1}$ as a function of the grid constant h on a double-logarithmic scale. Figures similar to this can be easily constructed for the four cases $\lambda = 0.005$, $\alpha = 4$ and $\alpha = 6$, and $\lambda = 0.01$, $\alpha = 4$ and $\alpha = 6$. The bisection-error (broken line) increases for small h values and is clearly related to the spike in the potential energy function. A careful analysis of table 1 reveals that in some cases the $E_i - E_{i+1}$ error estimate is below the bisection error. This is possible because the bisection iteration was continued after the estimated error bound was reached, which can give higher accuracy in some special cases (Wilkinson and Reinsch 1971).

Aguilera-Navarro *et al* (1990) have developed a series expansion for the ground state energy of a spiked harmonic oscillator, valid for large values of λ, $(2 \leqslant \lambda < \infty)$ and arbitrary values of α. Their expression reads

$$E_0 \simeq \left(1 + \frac{2}{\alpha}\right)\frac{1}{z}(1 + f_1 z + f_2 z^2 + f_3 z^3 + \ldots) \tag{2}$$

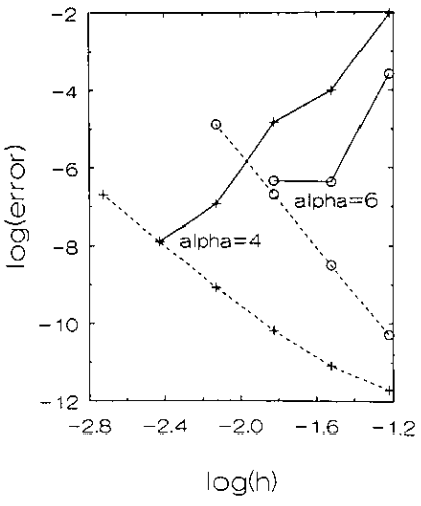

Figure 1. The error in the ground state eigenenergy of the spiked harmonic oscillator (equation (1), $\lambda = 0.0025$ and $\alpha = 4(+)$ and $\alpha = 6(^{\circ})$), as a function of the grid constant (h) using the tenth-order approximation for the Laplacian (full lines). The bisection error (broken lines) increases for small grid constants.

where $z = (2/\alpha\lambda)^{2/(\alpha+2)}$, and

$$f_1 = \frac{(\alpha+2)^{1/2}}{1+2/\alpha} \qquad f_2 = \frac{(\alpha+1)(8-\alpha)}{72(1+2/\alpha)} \qquad f_3 = \frac{(\alpha+1)(\alpha-2)(\alpha^2-\alpha-74)}{1728(\alpha+2)^{1/2}(1+2/\alpha)}.$$

The standard Padé approximant technique (Baker and Graves-Morris 1981, Cabannes 1975, Hioe 1977, Killingbeck 1985) has proved successful in reproducing the correct behaviour of functions for which only the beginning of an expansion series is available; the method has also been applied with success to cases where many (over 20) series coefficients are known, as in the critical phenomena associated with lattice-spin models (Gaunt and Guttmann 1974), or in several quantum problems (Čizek and Vrscay 1982). It appears that little work has been done to extract useful information from series bearing only a handful (4 to 5) of coefficients (Aguilera-Navarro and Estévez 1988, Aguilera-Navarro *et al* 1988, 1991).

In this paper, the simple, expeditious and inexpensive Padé approximants method is employed to extrapolate the four-term large coupling constant expansion for the energy given by (2), to a region far beyond that of its validity. The new expression thus found is only meant for the evaluation of the ground state energy of the spiked harmonic oscillator for arbitrary values of the coupling parameter λ. Thus we will not be concerned with the analytic manipulation of the function developed.

In the present work we employ the notation (M/N), to denote an Mth degree polynomial divided by an Nth degree polynomial. The only non-trivial, third-order Padé forms that can be constructed for the four-term quantity between parentheses in the energy expression (2) are (1/2), (2/1) and (0/3). From this triad of approximants one must be selected such that ideally it represents well the original large-coupling-constant expansion for the energy and is also reliable for $0 < \lambda \leqslant 2$. The results for the energy of the spiked harmonic oscillator obtained by using forms (0/3) and (1/2) were compared with the corresponding ones from the numerical integration of the radial equation employing the Lanczos/grid method. The numerical analysis performed

showed that the approximant (1/2) yielded positive values for the energy, as it ought, but that these values were always considerably lower than the exact ones. The Padé form (0/3) rendered negative (unphysical) values of the energy for $\lambda \leqslant 0.02$ regardless of the value of α. These are sufficient reasons to discard forms (0/3) and (1/2). The remaining form, (2/1), does not possess singularities in the range $0 \leqslant \lambda < \infty$. More importantly the approximation

$$E \simeq \left(1+\frac{2}{\alpha}\right)\frac{1}{z}(2/1)(z) \tag{3}$$

has been found to be highly accurate. For instance, for $\alpha = 4$ and $\lambda = 0.0025$ the relative error is $9.8 \times 10^{-2}\%$. When $\alpha = 6$ and $\lambda = 0.0025$ the error increases to $3.2 \times 10^{-1}\%$.

Employing a judicious blend of the theory of perturbations of linear operators, and approximation techniques for differential equations, Harrel (1977) has been able to derive explicit expressions for the lowest-order corrections to the eigenvalues of the spiked harmonic-oscillator Hamiltonian. The modified perturbation theory results due to Harrel are asymptotically correct for small values of λ. Harrel (1977) has proved that the ground state energy expressions for $\alpha = 4$ and $\alpha = 6$ correct to lowest order obey the algebraic forms

$$E_0(\alpha = 4, \lambda) = 3 + \frac{4}{\sqrt{\pi}}\lambda^{1/2} + O(\lambda) \tag{4}$$

$$E_0(\alpha = 6, \lambda) = 3 + \frac{8\Gamma(3/4)}{\sqrt{\pi}\Gamma(1/4)}\lambda^{1/4} + O(\lambda^{1/2}). \tag{5}$$

Unfortunately, the derivation of higher-order perturbative corrections to the eigenvalues given by (4) and (5) are likely to be exceedingly laborious. The values of the gamma function in equation (5) are $\Gamma(3/4) = 1.225\,4167$, and $\Gamma(1/4) = 3.625\,6099$.

Table 2 compares our results for the energy for the case $\alpha = 4$ with those of Detwiler and Klauder (1975), Harrel (1977) and Killingbeck (1982). The superscript d in the energy E represents the Padé extrapolation result given by (3). The numerical integration results of the Schrödinger equation employing the Lanczos/grid method are given in the last column. The latter results are in virtual perfect agreement with those found by Killingbeck (1982), employing the Richardson extrapolation technique (Richardson and Gaunt 1927, Joyce 1973); this lends further support to the conjecture of Killingbeck (1982) that there was some slight error in the computer program employed by Detwiler and Klauder (1975). Table 3 is the same as table 2 except that $\alpha = 6$.

Table 2. Some sample ground state energy eigenvalues for the spiked harmonic-oscillator Hamiltonian. All energies are displayed in arbitrary units. $\alpha = 4$.

λ	E^a	E(formula)^b	E^c	E^d	E(Lanczos)^e
0.01	3.205 27	3.075 22	3.205 07	3.204 42	3.205 067
0.005	3.148 39	3.053 19	3.148 35	3.146 64	3.148 352
0.0025	3.106 70	3.037 61	3.106 81	3.103 77	3.106 809

[a] From Detwiler and Klauder (1975).
[b] From Harrell (1977).
[c] From Killingbeck (1982). Richardson extrapolation.
[d] From the present work. Padé approximant technique.
[e] From the pressnt work. Lanczos/grid method.

Table 3. Same as table 2 except that $\alpha = 6$.

λ	E^a	E(formula)^b	E^c	E^d	E(Lanczos)^e
0.01	3.505 74	3.096 48	3.505 45	3.496 88	3.505 452
0.005	3.423 02	3.081 13	3.422 88	3.413 16	3.422 884
0.0025	3.353 95	3.068 22	3.353 92	3.343 05	3.353 919

For explanation of notes see table 2.

4. Results

Eigenenergies of the ground state of the spiked harmonic-oscillator Hamiltonian have been calculated for $\alpha = 4$ and $\alpha = 6$ and small values of the coupling parameter, i.e. $\lambda \leq 0.01$. The results for the eigenvalues obtained by integration of the Schrödinger equation using the Lanczos/grid method (1950) were compared to those obtained by Killingbeck (1982) employing the Richardson extrapolation (of finite difference results). The finite difference method for eigenvalues advocated by Killingbeck (1982, 1991) gives results which are very accurate, showing that this last simple and efficient procedure can be utilized with profit even for attractive real potentials with radial form more singular than the inverse square at the origin.

A small-coupling-constant series expansion in the parameter λ^ν ($\nu = \frac{1}{2}$ for $\alpha = 4$; $\nu = \frac{1}{4}$ for $\alpha = 6$) for the ground state energy of the spiked harmonic oscillator exists in the literature (Harrel 1977). In addition, there also exists a large-coupling-constant perturbative expansion (Aguilera-Navarro *et al* 1990). Since it would be of interest to derive an analytical expression applicable for intermediate values of the coupling parameter, we have constructed, with minimal labour, an approximant to represent the energy in this region; surprisingly, the single Padé extrapolant constructed, based on a large coupling series, was found to be far superior to the truncated series expansion. In fact, equation (3) for the ground state energy eigenvalues of the spiked harmonic-oscillator Hamiltonian never deviates from the exact results by more than one-half of 1% on $0 \leq \lambda < \infty$.

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