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THE VARIATIONAL SPIKED OSCILLATOR

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Abstract

A variational analysis of the spiked harmonic oscillator Hamiltonian $-d^2/dx^2 + x^2 + \lambda/|x|^{6/2}, \lambda > 0$, is reported in this work. A trial function satisfying Dirichlet boundary condition is suggested. The results are excelent for a large range of values of the coupling parameter λ.

1 Introduction

The so called spiked harmonic oscillator, defined by the hamiltonian

$$H = -\nabla^2 + r^2 + \lambda/r^\alpha, \tag{1}$$

has recently been object of studies in several papers [1]-[6]. One of its intrinsic importance stems from the necessity of adding a spiked term to the usual harmonic oscillator approximation near the minimum of a given short-range potential.

Several methods, most of them perturbative ones, were applied in order to obtain a description of the ground state for different interaction regimes — small and large coupling constant λ — and different degrees of singularities at the origin — characterized by the positive parameter α.

In Section 3, we carry out a variational analysis of the hamiltonian for the special case of $\alpha = 5/2$. From this values of α up, the hamiltonian becomes supersingular at the origin. It turns out that the variational analysis, using the bases introduced in this paper, leads to extremely good results for all values of λ, i.e., for weak, moderate and strong interactions.

2 Formulation of the problem

The 3D wave equation we have to deal with reads

$$\left[-\nabla^2 + r^2 + \lambda/r^\alpha\right] \psi(\vec{r}) = E\psi(\vec{r}). \tag{2}$$

The associated radial wave equation for the ground state reduces to

$$\left[-\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} + r^2 + \frac{\lambda}{r^\alpha}\right] R(r) = ER(r), \tag{3}$$

with $R(r)$ satisfying the usual boundary condition $R(r) \to 0$ as $r \to 0$ and the Dirichlet condition $R(0) = 0$. This radial function is normalized according to the condition

$$\int_0^\infty R^2(r) r^2 dr = 1. \tag{4}$$

Our variational function is defined as a linear combination of the basic functions

$$R_n(r) = A_n r^\beta M(-n, \beta + 3/2, r^2) e^{-r^2/2}, \quad n = 0, 1, 2, \ldots. \tag{5}$$

where $M(a, b, z)$ is a confluent hypergeometric function as defined, for instance, in Ref.[7].

In our trial base Eq.(5), β is a variational parameter to be determined. Obviously, β depends also on the dimension of the space where the variational analysis is carried out. As this parameter

λ	β	E_{calc}	E_{exact}	$error(\%)$
0.001	0.0426	3.004054	3.004022	0.001
0.010	0.03674	3.037846	3.036729	0.037
0.100	0.210460	3.273543	3.266873	0.204
1.000	0.8325298	4.325682	4.317311	0.194
10.00	2.7414613	7.740873	7.735111	0.074
100.0	8.19143095	17.546306	17.541889	0.025
1000.	23.42159139	44.959424	44.955485	0.009

Table 1: Energies obtained from Eq.(7) for $\alpha = 5/2$. E_{exact} refers to the energies obtained by numerical integration of the wave equation [2]. The *error* is defined by $100|E_{calc} - E_{exact}|/E_{exact}$.

is present in a nonlinear way, we should develop a discrete variational analysis on it. Instead, we preferred to determine it analitically considering only the first component $R_0(r)$ as the variational trial function.

In other words, the variational function

$$R(r) = A_0 r^{\beta} e^{-r^2/2}, \tag{6}$$

provides us with the ground-state energy

$$E = 3 + \frac{\Gamma(\beta - \alpha/2 + 3/2)}{\Gamma(\beta + 3/2)}\lambda + \frac{2\beta^2}{2\beta + 1}, \tag{7}$$

where, for given values of α and λ, the parameter β is determined from the implicit equation

$$\frac{2\beta(\beta+1)}{(2\beta+1)}\frac{\Gamma(\beta+1/2)}{\Gamma(\beta-\alpha/2+3/2)}\frac{1}{[\psi(\beta+3/2)-\psi(\beta-\alpha/2+3/2)]} = \lambda. \tag{8}$$

In Eq.(8), $\psi(z)$ is the usual psi (or digamma) function defined by the logarithmic derivative of the gamma function [7]

$$\psi(z) = \Gamma'(z)/\Gamma(z). \tag{9}$$

In Table 1, we display the values of β and the ground-state energy obtained from Eqs.(8) and (7), respectively, for several values of the coupling parameter λ, and $\alpha = 5/2$.

3 Normalization and matrix elements

In this Section, we consider the limit case of $\alpha = 5/2$, as previously mentioned in the Introduction. The normalization condition defined by Eq.(4) requires that the coefficientts A_n of Eq.(5) are given

by

$$A_n^2 = 2\Gamma(n+\beta+3/2)/n!\Gamma^2(\beta+3/2). \tag{10}$$

In order to get the matrix elements of the hamiltonian (1) in the basis (5), we conveniently split the hamiltonian of Eq.(3) in two terms as

$$H = H_0 + H_1, \tag{11}$$

where

$$H_0 = -\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} + r^2 + \frac{\beta(\beta+1)}{r^2}, \tag{12}$$

and

$$H_1 = \frac{\lambda}{r^{5/2}} - \frac{\beta(\beta+1)}{r^2}. \tag{13}$$

It can be seen easily that H_0 is diagonal in the basis $R_n(r)$ defined by Eq.(5) with eigenvalues given by

$$E_{0n} = 4n + 2\beta + 3. \tag{14}$$

The matrix elements of H_1 in the basis defined by Eq.(5) are given by

$$(H_1)_{nm} = \frac{1}{2}A_n A_m \left[\lambda S_{nm} - \beta(\beta+1)G_{nm}\right], \quad n, m = 0, 1, 2, \ldots, \tag{15}$$

with

$$S_{nm} \equiv S_{nm}(\beta) = \frac{\Gamma^2(\beta+3/2)}{\Gamma(n+\beta+3/2)} \sum_{q=0}^{m} (-1)^q \binom{m}{q} \frac{\Gamma(q+\beta+1/4)\Gamma(n+5/4-q)}{\Gamma(q+\beta+3/2)\Gamma(5/4-q)}, \tag{16}$$

and

$$G_{nm} \equiv G_{nm}(\beta) = \frac{n!\Gamma(\beta+3/2)\Gamma(\beta+1/2)}{\Gamma(n+\beta+3/2)}. \tag{17}$$

In the numerical calculations, it helps to realize that Eq.(16), for $m = 0$, reduces to

$$S_{n0} = \left(\frac{5}{4}\right)_n \frac{\Gamma(\beta+1/4)}{\Gamma(n+\beta+3/2)}, \tag{18}$$

where $(x)_n$ is a Pochhammer symbol as defined in Ref.[7]. It is also interesting to note that G_{nm} does not depend on m, *i.e.*, all matrix elements G_{nm} are equal in a given row.

It is easy to verify that Eqs.(14) and (15) with $m = n = 0$ reproduce the "zero-quantum energy" given in Eq.(7) when $\alpha = 5/2$.

λ	β	E_1	E_2	E_4	E_6	E_8	E_{10}	E_{exact}
0.001	0.0426	3.00680	3.00583	3.00521	3.00496	3.00481	3.00471	3.00402
0.010	0.03674	3.03785	3.03773	3.03769	3.06768	3.03768	3.03768	3.03673
0.100	0.210460	3.27354	3.27225	3.27199	3.27199	3.27198	3.27195	3.26687
1.000	0.8325298	4.32568	4.32370	4.32359	4.32310	4.32252	4.32199	4.31731
10.00	2.7414613	7.74087	7.73982	7.73820	7.73677	7.73603	7.73565	7.73511
100.0	8.19143095	17.54631	17.54589	17.54268	17.54201	17.54191	17.54189	17.54189
1000.	23.42159139	44.95942	44.95927	44.95560	44.95549	44.95549	44.95549	44.95549

Table 2: Energies and convergence of the method for a large range of values for the coupling parameter λ. E_D refers to the variational energy in the sub-space of dimension D. E_{exact} refers to the energies obtained by numerical integration of the wave equation [2].

4 Results and comments

The variational analysis was carried out in a 10-dimensional space. The diagonalization of the hamiltonian was also made in subspaces in order to get an idea of the trend of the method. The results for the values of λ given in Table 1 are displayed in Table 2. The diagonalizations were carried out with an accuracy of 6 decimal digits. However, for sake of space, only five digits are shown. The entries E_{exact}, obtained through numerical integration of the wave equation, were taken from Ref.[2].

A simplification we imposed in our calculations was to take the relationship between β and λ from Eq.(8), for $\alpha = 5/2$. As mentioned in Section 2, this relationship was determined via a "zero-quantum" calculation. A better analysis would be to determine β in each subspace where the variational analysis is being carried out. However, the expected improvements woult not justify the extra numerical work involved face the excelent results already obtained in the very large range of values for the coupling constant λ, and displayed in Table 2. The variational energies determine upper bounds to the ground-state ones in accordance to the variational theorem. The remarkable agreement with E_{exact} for all values of the parameter λ suggests that the trial function used must have a very good overlap to the exact eigenfunction.

References

[1] E. M. Harrell, Ann. Phys. (N.Y.) 105, 379 (1977).

[2] V. C. Aguilera-Navarro, G. A. Estévez and R. Guardiola, J. Math. Phys. 31, 99 (1990).

[3] V. C. Aguilera-Navarro and R. Guardiola, J. Math. Phys. 32, 2135 (1991).

[4] R. Guardiola and J. Ros, J. Phys. A: Math. Gen. 25, 13551 (1992).

[5] V. C. Aguilera-Navarro, Francisco M. Fernández, R. Guardiola and J. Ros, preprint FTUV/92-18, (1992) *Departamento de Física Atómica y Nuclear, Universidad de Valencia, Valencia, 46100 Spain.*

[6] M. Znojil, Phys. Letters A 164, 138 (1992).

[7] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1970).