International Journal of Theoretical Physics, Vol. 33, No. 8, 1994

Variational Spiked Oscillator

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Received August 31, 1993

A variational analysis of the spiked harmonic oscillator Hamiltonian $-d^2/dr^2 + r^2 + \lambda/r^{5/2}$, $\lambda > 0$, is reported. A trial function automatically satisfying both the Dirichlet boundary condition at the origin and the boundary condition at infinity is introduced. The results are excellent for a very large range of values of the coupling parameter λ, suggesting that the present variational function is appropriate for the treatment of the spiked oscillator in all its regimes (strong, moderate, and weak interactions).

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 an object of study (Harrell, 1977; de Llano, 1981; Aguilera-Navarro *et al.*, 1990, 1992; Aguilera-Navarro and Guardiola, 1991; Fernández, 1991; Znojil, 1991, 1992; Guardiola and Ros, 1992; Solano-Torres *et al.*, 1992). One aspect of its intrinsic importance stems from the necessity of adding a spiked term to the generally used harmonic oscillator approximation near the minimum of a given short-range potential.

Several methods were tried in order to obtain a description of the ground state for different interaction regimes—small, moderate, and large coupling constant λ—and different degrees of singularities at the origin—characterized by the positive parameter α. In general, each of these interaction regimes requires a different and specific treatment, usually requiring perturbation schemes.

In Section 2, we formulate explicitly the problem and introduce a variational function that satisfies the Dirichlet boundary condition at the origin and has the appropriate behavior at infinity.

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0020-7748/94/0800-1673$07.00/0

In Section 3, we carry out a variational analysis of the Hamiltonian for the special case of $\alpha = 5/2$. 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 at once. The results obtained in variational spaces of different dimensions are compared with the values obtained by numerically integrating the Schrödinger equation and reported in Aguilera-Navarro *et al.* (1990). It results that in a ten-dimensional variational space the highest "error" is of the order of only 0.16%. Other results and comments are presented in the last section.

2. FORMULATION OF THE PROBLEM

The 3D wave equation we have to deal with reads

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

The associated radial wave equation for the ground state reduces to

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

complemented with the usual boundary condition $R(r) \to 0$ as $r \to \infty$ and the Dirichlet condition $R(0) = 0$. The 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

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

where $M(a, b, z)$ is a confluent hypergeometric function as defined, for instance, in Abramowitz and Stegun (1970). As n is an integer, the hypergeometric function reduces to a polynomial. Consequently, every function $R_n(r)$ satisfies the above boundary conditions.

In our trial base equation (5), β is a variational parameter to be determined. Besides depending on λ and α, β depends also on the dimension of the space where the variational analysis is carried out. As this parameter is present in a nonlinear way, we should develop a discrete variational analysis on it. Instead, we prefer to follow a different procedure. By considering only the first component $R_0(r)$ as the variational trial function, we are able to determine the parameter β analytically. In other words, the variational function

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

and the radial equation (3) provide us with the variational 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 equation (8), $\psi(z)$ is the usual psi (or digamma) function defined by the logarithmic derivative of the gamma function (Abramowitz and Stegun, 1970)

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

In Table I, we display the values of β and the ground-state energy obtained from equations (8) and (7), respectively, for several values of the coupling parameter λ, and $\alpha = 5/2$. The values of β associated with each λ value are taken from this table and used in the next section to carry out a more extensive variational analysis.

3. NORMALIZATION AND MATRIX ELEMENTS

In this section, we consider the special limiting case of $\alpha = 5/2$ and develop a variational analysis of the Hamiltonian (3) with the basic functions (5). Varying the dimension of the variational space, we can see the trend of the method. It results that the convergence is extremely fast for all values of the interaction parameter λ in the ample range of values considered.

Table I. Energies Obtained from Equation (7) for $\alpha = 5/2$[a]

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
10.000	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

[a] E_{exact} refers to the energies obtained by numerical integration of the wave equation as reported in Aguilera-Navarro *et al.* (1990). The error is defined by $100|E_{\text{calc}} - E_{\text{exact}}|/E_{\text{exact}}$. The values of β were obtained from equation (8) with $\alpha = 5/2$.

The normalization condition defined by equation (4) requires that the coefficients A_n of equation (5) be 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 (3) in the basis (5), we conveniently split that operator into 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 equation (5). Its eigenvalues E_{0n} are given by

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

On the other hand, the matrix elements of H_1 in the basis defined by equation (5) are given by

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

with

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

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 equation (16) for $m = 0$ reduces to

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

Table II. Energies and Convergence of the Method for a Large Range of Values for the Coupling Parameter λ[a]

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	3.03768	3.03768	3.03768	3.03763
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

[a] E_D refers to the variational energy in the subspace of dimension D; E_{exact} refers to the energies obtained by numerical integration of the radial wave equation as reported in Aguilera-Navarro *et al.* (1990).

where $(z)_n$ is a Pochhammer symbol as defined in Abramowitz and Stegun (1970). 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 equations (14) and (15) with $m = n = 0$ reproduce the "zero-quantum energy" given in equation (7) when $\alpha = 5/2$.

4. RESULTS AND COMMENTS

The variational analysis was carried out in a ten-dimensional space. The diagonalization of the Hamiltonian was also made in several subspaces in order to get an idea of the trend of the method. The results for the values of λ given in Table I are displayed in Table II. It can be noted that the convergence of the method is very fast. The diagonalizations were carried out with an accuracy of six 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 Aguilera-Navarro *et al.* (1990).

A simplification we imposed in our calculations was to take the relationship between β and λ from equation (8) for $\alpha = 5/2$. As explained in Section 2, this relationship was determined via a "zero-quantum" calculation. In principle, a better analysis would be to determine β in each subspace where the variational analysis is being carried out. However, the expected improvements would not justify the extra numerical work involved, in view of the excellent results already obtained in the very large range of values for the coupling constant λ and displayed in Table II. The variational energies determine upper bounds to the exact ground-state ones in accordance with 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.

Finally, we must stress that we were able to treat the spiked harmonic oscillator in *all* its regimes, namely under weak, moderate, and strong coupling, at once. Other methods require special adaptations to deal with each of these regimes separately.

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