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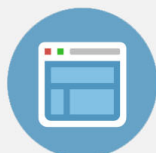
Variational and perturbative schemes for a spiked harmonic oscillator

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A variational analysis of the spiked harmonic oscillator Hamiltonian operator $-d^2/dx^2 + x^2 + l(l+1)/x^2 + \lambda |x|^{-\alpha}$, where α is a real positive parameter, is reported in this work. The formalism makes use of the functional space spanned by the solutions of the Schrödinger equation for the linear harmonic oscillator Hamiltonian supplemented by a Dirichlet boundary condition, and a standard procedure for diagonalizing symmetric matrices. The eigenvalues obtained by increasing the dimension of the basis set provide accurate approximations for the ground state energy of the model system, valid for positive and relatively large values of the coupling parameter λ. Additionally, a large coupling perturbative expansion is carried out and the contributions up to fourth-order to the ground state energy are explicitly evaluated. Numerical results are compared for the special case $\alpha = 5/2$.

I. INTRODUCTION

A general problem connected with the so-called spiked harmonic oscillator (SHO) Hamiltonian $-d^2/dx^2 + x^2 + l(l+1)/x^2 + \lambda |x|^{-\alpha}$, where α is a positive constant, has been thoroughly studied by Harrell.[1] The name spiked derives from the graphical appearance of the perturbative term $\lambda |x|^{-\alpha}$. The quantity λ is a positive definite parameter and measures the strength of the perturbative potential. The angular momentum term is represented by the expression $l(l+1)/x^2$. The spiked harmonic oscillator problem is of practical importance as it occurs in both chemical and nuclear physics.[1-7] In the elegant work reported in Ref. 1, a modified perturbation series to a finite order is employed to obtain analytical expressions for the eigenenergies of a SHO Hamiltonian for small values of λ, and arbitrary values of the exponent α. In this work, we report attempts to solve the SHO problem, employing a variational procedure and a large coupling perturbative calculation. A short review of the SHO problem is presented in Sec. II. The variational approach is outlined in Sec. III. The large coupling expansion is discussed and developed in Sec. IV, and a summary of the results and conclusions is found in Sec. V.

II. BACKGROUND

To compare our results with those reported by Harrell,[1] we concentrate ourselves on the zero angular momentum case. The Hamiltonian associated with the SHO then reads

$$H(\alpha,\lambda) = \frac{-d^2}{dx^2} + x^2 + \lambda |x|^{-\alpha} \equiv H_0 + \lambda V, \qquad (2.1)$$

where H_0 is formally equal to the simple harmonic oscillator Hamiltonian, and $V = |x|^{-\alpha}$. The sum of H_0 and λV must be understood to be the Friedrichs extension of the quadratic form defined by Eq. (2.1) on the domain of the Schwartz space with the boundary condition $u(0) = 0$, with $u(x)$ de-

noting a solution of the Schrödinger equation for the simple harmonic oscillator. The latter condition is necessary since not all functions in the domain of H_0 are in the domain of V. Therefore, when $\lambda \to 0$, α fixed, the operator $H(\alpha,\lambda)$ converges to an operator formally equal to $-d^2/dx^2 + x^2$, but supplemented by the Dirichlet boundary condition (DBC) that all functions in its domain vanish at $x = 0$. This operator is H_0. With this definition, the family of operators $H(\alpha,\lambda)$ is both analytic for $\lambda > 0$, and continuous for $\lambda \to 0^+$.

The spectrum of H_0 consists of the (two-fold degenerate) simple harmonic oscillator eigenvalues, whose eigenfunctions vanish at $x = 0$. Since one purpose of the present work is to consider the perturbation expansion of the eigenvalues of $H(\alpha,\lambda)$, all operators will be restricted to the space $L^2[0,\infty]$, with the DBC $u(0) = 0$, to avoid problems stemming from the degeneracy of the spectrum.

As has been pointed out elsewhere, the perturbation V considered in this article is singular.[1,4-6] The series expansion for the eigenvalues $E_n(\alpha,\lambda)$ of $H_0 + \lambda V$, calculated by means of the Rayleigh–Schrödinger procedure, yields divergent expressions for the second- and higher-order perturbative corrections. Harrell[1] has thus utilized an improved perturbation scheme to obtain corrections for order greater than unity for the eigenvalues. For instance, his expression for the SHO ground state energy and for $\alpha = 5/2$ reads,[1]

$$E_0\left(\frac{5}{2},\lambda\right) = 3 + \frac{2\Gamma(1/4)}{\Gamma(1/2)}\lambda$$
$$+ \frac{16}{\Gamma(1/2)}\lambda^2 \ln\lambda + O(\lambda^2). \qquad (2.2)$$

In the expression above, we have corrected for a misprint in the sign of the log term.

The presence in Eq. (2.2) of an explicit term between first and second orders in λ should be mentioned. This equation, valid for small values of the coupling parameter λ, is strikingly similar to the expansion for the ground state ener-

gy per particle for a boson system.[8] An alternative scheme will be employed in the present work to obtain corrections to $E_0(\alpha,\lambda)$. The methodology followed here is well known and is briefly presented in the next sections.

III. THE VARIATIONAL APPROACH

In the variational approach, the first step is to choose a complete set of basis functions. Although in principle one can employ an arbitrary basis of sufficiently smooth functions, in numerical practice the rate of convergence for singular problems depends a great deal on how the basis is chosen. The more clever one is in choosing a set of functions, the faster the convergence of the method. In this article, we take the basis set constructed with the normalized solutions of the Schrödinger equation for the linear harmonic oscillator with a DBC, i.e., the harmonic oscillator eigenfunctions $u(x)$ normalized in the interval $0 \leq x < \infty$, with the prescription that $u(0) = 0$. As is well known, these energy eigenfunctions are essentially the product of Hermite polynomials of odd degree with a Gaussian function. We write

$$\langle x|n\rangle \equiv u_n(x) = A_n e^{-x^2/2} H_{2n+1}(x), \quad n = 0,1,2,..., \tag{3.1}$$

A_n being a normalizing factor. The functions $u_n(x)$ define a complete orthonormal set of solutions of H_0 in the interval $0 \leq x \leq \infty$, with

$$A_n^{-2} = 4^n(2n+1)!\Gamma(1/2). \tag{3.2}$$

Now, let $\varphi(x)$ be an eigenfunction of the SHO Hamiltonian (1), and let us expand $\varphi(x)$ in terms of $u_n(x)$, namely,

$$\varphi(x) = \sum_{n=0}^{\infty} a_n u_n(x). \tag{3.3}$$

Next, we want to minimize the eigenenergies of (2.1), with respect to the variational parameters a_n, $n = 0,1,...,N-1$, in the finite dimensional subspace spanned by the N functions $u_0, u_1,...,u_{N-1}$. This variational problem is equivalent to diagonalizing the Hamiltonian (2.1) in the chosen basis representation. By varying the dimension N, we get the trend of the method.

All we need is to evaluate the matrix elements of $H(\alpha,\lambda)$ in the basis (3.1). They can be separated into two contributions ($\beta \equiv -\alpha$),

$$H_{m+1,n+1}(\alpha,\lambda) \equiv \langle m|H_0|n\rangle + \lambda \langle m|x^\beta|n\rangle,$$
$$m,n = 0,1,...,N-1. \tag{3.4}$$

Since H_0 is diagonal in the chosen basis, we see that the first term on the right hand side of Eq. (3.4) is simply the expression for the energy eigenvalues of the harmonic oscillator with DBC, that is,

$$\langle m|H_0|n\rangle = (4n+3)\delta_{m,n}, \quad m,n = 0,1,2,...,N-1. \tag{3.5}$$

Alternative procedures exist for deriving the matrix elements of the operator x^β appearing in (3.4). A direct way we develop here is to use the following representation for the odd-degree Hermite polynomials,

$$H_{2n+1}(x) = \frac{(-1)^n(2n+1)!\Gamma(1/2)}{n!}$$
$$\times \sum_{m=0}^{n} (-1)^m \binom{n}{m} \frac{x^{2m+1}}{\Gamma(m+3/2)}. \tag{3.6}$$

The desired result, which involves finite double summations, reads

$$\langle m|x^\beta|n\rangle = T_m T_n \Gamma(3/2)$$
$$\times \sum_{k=0}^{m} \sum_{l=0}^{n} (-1)^{k+l} \binom{m}{k}\binom{n}{l}$$
$$\times \frac{\Gamma[k+l+(\beta+3)/2]}{\Gamma(k+3/2)\Gamma(l+3/2)}, \tag{3.7}$$

with

$$T_s \equiv (-1)^s \sqrt{(2s+1)!}/2^s s!. \tag{3.8}$$

Equation (3.7) is simple enough to be used in practical applications. However, it may be still reduced by carrying out explicitly one of the sums, e.g., the sum over l. The relevant terms for this sum are

$$S = \sum_{l=0}^{n} (-1)^l \binom{n}{l} \frac{\Gamma(l+u)}{\Gamma(l+3/2)}, \tag{3.9}$$

where $u = k + (\beta+3)/2$. Now we note that the binomial coefficient can be expressed as

$$\binom{n}{l} = (-1)^l(-n)_l/l!,$$

where $(-n)_l$ is the Pochhammer symbol.[9] Moreover, $\Gamma(l+z) = \Gamma(z)(z)_l$, so that (3.9) is the same as

$$S = \frac{\Gamma(u)}{\Gamma(3/2)} \sum_{l=0}^{n} \frac{1}{l!} \frac{(-n)_l(u)_l}{(3/2)_l}. \tag{3.10}$$

As n is integer, the sum in (3.10) corresponds to the hypergeometric function $_2F_1(-n,u;3/2;1)$ which has a very simple known expression.[9] Thus we can write (3.10) as

$$S = \frac{\Gamma[k+(\beta+3)/2]\Gamma(n-k-\beta/2)}{\Gamma(n+3/2)\Gamma(-k-\beta/2)}. \tag{3.11}$$

Finally, the matrix element of interest is given by

$$\langle m|x^\beta|n\rangle = T_m T_n \frac{\Gamma(3/2)}{\Gamma(n+3/2)}$$
$$\times \sum_{k=0}^{m} (-1)^k \binom{m}{k}$$
$$\times \frac{\Gamma[k+(\beta+3)/2]\Gamma(n-k-\beta/2)}{\Gamma(k+3/2)\Gamma(-k-\beta/2)}, \tag{3.12}$$

where the sum can be shown to be a polynomial of degree $m+n$ in β. A case of particular interest is the matrix element $\langle 0|x^\beta|n\rangle$ which, after some trivial algebra, reduces to

$$\langle 0|x^\beta|n\rangle = \frac{1}{\sqrt{(2n+1)!}} \frac{\Gamma[(\beta+3)/2]}{\Gamma(3/2)}$$
$$\times \beta(\beta-2)\cdots(\beta-2n+2), \quad n = 1,2,... . \tag{3.13}$$

Equation (3.12) is an exact closed form expression for the matrix elements of the operator x^β in the simple harmon-

ic oscillator representation supplemented by DBC. Explicit forms of the first few matrix elements of x^β are given in the Appendix. The same procedure leads to similar closed form expression for the matrix elements of x^β in the regular harmonic oscillator representation.

IV. LARGE COUPLING EXPANSION

The idea behind the large coupling expansion is to consider the potential

$$V(x) = x^2 + \lambda x^{-\alpha} \qquad (4.1)$$

and Taylor expand it around its minimum. Let x_m and V_m be the values of x and $V(x)$, respectively, at the minimum. It is easy to see that

$$x_m = (\lambda \alpha/2)^{1/(\alpha+2)} \qquad (4.2)$$

and

$$V_m = \lambda^{2/(\alpha+2)} [(\alpha/2)^{2/(\alpha+2)} + (2/\alpha)^{\alpha/(\alpha+2)}]. \qquad (4.3)$$

Let $z = x - x_m$. The expansion of $V(x)$ around $z = 0$ can be written as

$$V(z) = V_m + (\alpha+2)z^2 + \sum_{k=3}^{\infty} (-1)^k \frac{2}{\alpha}(\alpha)_k \mu^{k-2} \frac{z^k}{k!}, \qquad (4.4)$$

where $(\alpha)_k$ is the Pochhammer symbol[9] and

$$\mu = (2/\lambda\alpha)^{1/(\alpha+2)}. \qquad (4.5)$$

Now let us rewrite the Schrödinger equation as

$$\left[\frac{-d^2}{dz^2} + V(z) \right] y = Ey. \qquad (4.6)$$

The zero-order contribution to E is given by

$$E_0 = V_m = (1 + 2/\alpha)\mu^{-2} \qquad (4.7)$$

and the next contribution comes from a harmonic oscillator in z, characterized by the energy parameter

$$\omega = \sqrt{a+2}. \qquad (4.8)$$

Thus, in the large coupling expansion method we have

$$E(\mu) = (1 + 2/\alpha)\mu^{-2} + (\alpha+2)^{1/2}$$
$$+ \text{higher-order terms in } \mu. \qquad (4.9)$$

For the particular case $\alpha = 5/2$, we have

$$E(\lambda) = \frac{9}{5}\left(\frac{5}{4}\right)^{4/9}\lambda^{4/9} + \left(\frac{9}{2}\right)^{1/2} + \cdots. \qquad (4.10)$$

Numerical results for several values of λ are displayed in Table I.

The higher-order contributions can be obtained through a special perturbation expansion as shown in the following discussion. Consider

$$H = H_0 + \sum_{n=1}^{\infty} \mu^n H_n, \qquad (4.11)$$

with,

$$H_0 = \frac{-d^2}{dz^2} + \omega^2 z^2 + V_m, \qquad (4.12)$$

where, as before, $z = x - x_m$, and V_m and ω are given by (4.3) and (4.8), respectively. In (4.11), H_n is given by

$$H_{m-2} = (-1)^m (2/\alpha)(\alpha)_m (z^m/m!) \qquad (4.13)$$

with μ, defined in (4.5), playing the role of a coupling constant.

Now, as usual, set

$$E(\mu) = E_0 + \mu E_1 + \mu^2 E_2 + \cdots \qquad (4.14)$$

TABLE I. Ground state energy eigenvalues of the spiked harmonic oscillator for $\alpha = 5/2$. The superscripts in the energy E denote the dimension of the harmonic oscillator basis set (supplemented by Dirichlet boundary condition) employed for diagonalizing the matrix of the energy operator defined by Eq. (3.4). Also shown are the energies obtained from Eq. (4.10) and from fourth-order large coupling perturbative calculation Eq. (4.33). For comparison, the values obtained from Ref. 1 and from numerical integration of the corresponding Schrödinger equation, labeled "Exact," are also tabulated. All energies are displayed in arbitrary units.

λ	$E^{(1)}$	$E^{(2)}$	$E^{(10)}$	$E^{(20)}$	Large coupling expansion	4th order perturbation	Ref. 1	Exact
0.001	3.004 091	3.004 086	3.004 078	3.004 075	$\cdots$	$\cdots$	3.004 028	3.004 022
0.005	3.020 455	3.020 346	3.020 148	3.020 071	$\cdots$	$\cdots$	3.019 259	3.019 142
0.01	3.040 910	3.040 475	3.039 701	3.039 409	$\cdots$	$\cdots$	3.036 753	3.036 729
0.05	3.204 553	3.193 800	3.177 840	3.172 753	$\cdots$	$\cdots$	3.136 946	3.152 429
0.1	3.409 106	3.366 866	3.316 061	3.302 485	2.835 650	$\cdots$	3.201 251	3.266 873
0.5	5.045 531	4.216 199	3.919 691	3.882 167	3.581 992	3.860 533	3.481 265	3.848 553
1	7.091 062	4.688 097	4.354 247	4.329 449	4.108 987	4.323 602	$\cdots$	4.317 311
5	23.455 313	6.304 223	6.297 319	6.296 712	6.185 725	6.297 553	$\cdots$	6.296 472
10	43.910 626	7.951 033	7.735 637	7.735 136	7.652 122	7.735 582	$\cdots$	7.735 111
100	412.106 269	36.802 319	17.541 891	17.541 890	17.511 104	17.541 916	$\cdots$	17.541 889
1000	4094.062 688	324.897 482	44.967 048	44.955 485	44.944 307	44.955 486	$\cdots$	44.955 485

$$\psi(\mu) = \psi_0 + \mu\psi_1 + \mu^2\psi_2 + \cdots . \qquad (4.15)$$

From

$$H\psi(\mu) = E_\mu \psi(\mu) \qquad (4.16)$$

and collecting terms in powers of μ, we get

$$\sum_{m=0}^{n} H_m \psi_{n-m} = \sum_{m=0}^{n} E_m \Psi_{n-m}, \quad n = 0,1,2\dots . \qquad (4.17)$$

To solve this hierarchy of equations, let us project on the complete basis $|N\rangle$ generated by the harmonic oscillator eigenvalue problem

$$H_0|N\rangle = \left(\frac{-d^2}{dz^2} + \omega^2 z^2 \right)|N\rangle$$

$$= e_N|N\rangle, \quad N = 0,1,2,\dots . \qquad (4.18)$$

The solution to (4.18) is well known and given by

$$|N\rangle = \left(\frac{1}{N!2^N}\right)^{1/2}\left(\frac{\omega}{\pi}\right)^{1/4} e^{-\omega z^2/2} H_N(\sqrt{\omega}z), \qquad (4.19)$$

with

$$e_N = 2\omega(N + 1/2), \qquad (4.20)$$

where H_N is a Hermite polynomial normalized in the interval $-\infty \leqslant z \leqslant \infty$. Moreover, Eqs. (4.17) are to be supplemented by the following orthogonality conditions

$$\langle\psi_0|\psi_0\rangle = 1 \text{ and } \langle\psi_0|\psi_n\rangle = 0, \quad \text{for } n > 0. \qquad (4.21)$$

The energy expression is obtained by projecting (4.17) on $|\psi_0\rangle \equiv |0\rangle$. In doing so, we get

$$E_n = \sum_{m=0}^{n-1} \langle 0|H_{n-m}|\psi_m\rangle, \quad n = 1,2,\dots . \qquad (4.22)$$

From parity considerations, it can be seen that E_1 (as well as any E_{2n+1}) vanishes. So, the first high-order contribution comes from E_2 and is given by

$$E_2 = \langle 0|H_2|0\rangle + \langle 0|H_1|\psi_1\rangle \qquad (4.23)$$

with H_1 and H_2 given by (4.13). The first contribution to E_2 is easily calculated. To evaluate the second one, we need to express $|\psi_1\rangle$ in terms of the basis functions $|N\rangle$. To do this, let us first project (4.17) on $|N\rangle$. From

$$\sum_{m=0}^{n} \langle N|H_m - E_m|\psi_{n-m}\rangle = 0, \qquad (4.24)$$

it is straightforward to obtain that ($N \neq 0, n = 1,2,\dots$)

$$\langle N|\psi_n\rangle = \frac{1}{2N\omega} \sum_{m=1}^{N} \sum_p \langle N|E_m - H_m|p\rangle\langle p|\psi_{n-m}\rangle, \qquad (4.25)$$

where p runs over the complete set (4.19). For $n = 1$, we get

$$\langle N|\psi_1\rangle = \frac{(\alpha+1)(\alpha+2)}{6N\omega} \langle N|z^3|0\rangle, \qquad (4.26)$$

which tells us that the only possibilities for N are $N = 1$ and $N = 3$, as in (4.26) we have harmonic oscillator matrix elements. These can be easily obtained through direct calculations. The results are

$$\langle 0|z^3|1\rangle = (9/8\omega^3)^{1/2}, \qquad (4.27)$$

$$\langle 0|z^3|3\rangle = (6/8\omega^3)^{1/2}. \qquad (4.28)$$

Thus, from (4.26) and the results above, we obtain

$$|\psi_1\rangle = \frac{(\alpha+1)(\alpha+2)}{18\omega(8\omega^3)^{1/2}} [9|1\rangle + \sqrt{6}|3\rangle]. \qquad (4.29)$$

Going back to (4.23), we see that to get the contribution E_2 we need the following harmonic oscillator matrix elements

$$\langle 0|H_2|0\rangle = (\alpha+1)(\alpha+2)(\alpha+3)/16\omega^2, \qquad (4.30a)$$

$$\langle 0|H_1|1\rangle = -(\alpha+1)(\alpha+2)/(8\omega^3)^{1/2}, \qquad (4.30b)$$

$$\langle 0|H_1|3\rangle = -\sqrt{6}(\alpha+1)(\alpha+2)/3(8\omega^3)^{1/2}. \qquad (4.30c)$$

Thus, using (4.8) we get the total second-order contribution

$$\mu^2 E_2 = (2/\lambda\alpha)^{2/(\alpha+2)}(\alpha+1)(8-\alpha)/72. \qquad (4.31)$$

The calculation of the next correction is quite involved, because of the long emerging expression to be manipulated. We have used a (deceptively simple) algorithm using the symbolic manipulation package SMP[10] to get the next E_4 correction. We ran out of memory when trying to evaluate E_6. The contribution is given by

$$\mu^4 E_4 = \frac{(\alpha+1)(\alpha-2)(\alpha^2-\alpha-74)}{1728(2+\alpha)^{1/2}} \cdot \left(\frac{2}{\lambda\alpha}\right)^{4/(\alpha+2)}, \qquad (4.32)$$

and putting everything together we finally obtain, for $\alpha = 5/2$,

$$E(\lambda) = \frac{9}{5}\left(\frac{5\lambda}{4}\right)^{4/9} + \left(\frac{9}{2}\right)^{1/2} + \frac{77}{288}\left(\frac{4}{5\lambda}\right)^{4/9}$$

$$- \frac{1967}{27648}\left(\frac{2}{9}\right)^{1/2}\left(\frac{4}{5\lambda}\right)^{8/9} + \cdots . \qquad (4.33)$$

Numerical results for several values of λ are displayed in Table I.

To go further we must abandon algebraic methods and use some kind of seminumerical algorithm. The hierarchy of equations (4.22) and (4.25) can be quite easily coded in FORTRAN, in order to obtain the value of the amplitudes $\langle N|\psi_n\rangle$ for a given value of α and subsequently the corresponding energy corrections E_{n+1} in a chained way. Note that in order to obtain E_{n+1} we require all wavefunctions $\psi_0,\psi_1,\dots,\psi_n$, but to obtain $\langle N|\psi_{n+1}\rangle$ we need the value of E_{n+1}. The calculation does not involve any approximation, aside from rounding errors. The values of the first twenty coefficients of the expansion corresponding to $\alpha = 5/2$ are displayed in Table II. The notation is such that the energy $E(\lambda)$ is given by

TABLE II. Coefficients for the large coupling perturbation expansion equation (4.34), for $\alpha = 5/2$.

n	E_n
2	0.267 361 111
4	−0.033 537 785
6	−0.017 395 489
8	0.011 679 410
10	0.001 109 577
12	−0.006 825 514
14	0.002 542 598
16	0.008 178 874
18	−0.011 093 142
20	−0.014 427 769

$$E(\lambda) = \frac{9}{5}\left(\frac{5\lambda}{4}\right)^{4/9} + \left(\frac{9}{2}\right)^{1/2} + \sum_{\substack{n=2 \\ (\text{even})}} E_n \left(\frac{4}{5\lambda}\right)^{2n/9}.$$

(4.34)

Here, E_n behaves quite erratically with n, and probably this is not a well behaved series expansion. When λ is large enough, say larger than 2, one can expect to get very precise results from the expansion. However, $\lambda = 4/5$ is certainly outside the convergence radius, if such radius exists.

One can try to understand this strange behavior. The large coupling perturbation method expands both interaction and wavefunction around the classical minimum of the potential, extending the new coordinate $z = x - x_m$ to the full real axis. Certainly the region $(-\infty, 0]$ is spurious because of the mere statement of the problem. When λ is large, the minimum is placed at a large value of x, so that the harmonic oscillator wavefunctions centered at x_m will not penetrate too much into the forbidden region. Obviously this is not the case for small λ. Probably the proper way of controlling this unwanted characteristic is to change variables to a new coordinate extending along the full real axis and carry out afterwards the large coupling perturbative expansion.

V. NUMERICAL RESULTS AND CONCLUSION

Since it is of some interest to have an idea of the relative size of the ground state spiked harmonic oscillator energies as the potential parameter increases, we have numerically integrated the Schrödinger equation. The exponent α was fixed at 5/2 to compare with Harrell's result Eq. (2.2). The energies so obtained are displayed in Table I under the entry "Exact."

From the computational point of view it resulted in a quite complex problem. First of all, because of the singular character of the potential near the origin, we could not use a small error integration formula, like, e.g., Numerov's method.[11] Instead, we had to use the lowest order approximation to the second derivative

$$D^2 = \delta^2/h^2,$$

where δ^2 represents the second-order centered differences, and h is the mesh spacing. Nevertheless, the results could be improved and tested by means of the Richardson extrapolation algorithm. To give an idea of the numerical difficulties, let us mention that to obtain the energy for $\lambda = 0.001$ with six decimal places, we had to use a mesh with 80 000 points.

From Eqs. (3.4), (3.5), and (3.7) and the results given in the Appendix, it can be readily seen that the first variational approximation (subspace of dimension 1) to the ground state eigenenergy of the SHO is

$$E^{(1)} = H_{11} = \langle 0|H|0\rangle = 3 + \lambda\Gamma\left[\frac{(\beta+3)}{2}\right]\Big/\Gamma(3/2),$$

(5.1)

which coincides with the $0(\lambda)$ correction of Harrell, Eq. (2.2).

When $N = 2$ the diagonalization can also be easily performed analytically, via the secular equation approach, and we have

$$E^{(2)} = \frac{1}{2}\Bigg[10 + \frac{53}{24}\lambda\gamma$$
$$\pm \left(16 + \frac{5}{3}\lambda\gamma + \frac{2425}{576}\lambda^2\gamma^2 \right)^{1/2} \Bigg].$$

(5.2)

From this expression, we notice that when the spikelike perturbation vanishes $(\lambda = 0)$, the two eigenvalues become 3 and 7, as expected.

For higher values of N we have to resort to numerical diagonalization procedures and we employed the known Jacobi method. Table I shows the convergence of the results for the ground state energy of the SHO, for selected values of λ, as the dimension of the basis set is increased.

To analyze the results of the variational calculation it is convenient to distinguish among three cases, corresponding to a) large values of the coupling constant $(\lambda \gtrsim 10)$; b) small values of $\lambda(<0.1)$; and c) medium values $(\lambda \simeq 1)$.

For large λ the calculations involving few basis states are definitely poor, but very good results are obtained when the basis space is enlarged (dimension 10 or more). In this region of λ, the variational method converges quite rapidly to the exact results.

In the case of very small λ, one can get the wrong impression that the variational method behaves properly. Just to clarify the previous statement let us consider the number 3.004 075 which appears in the column labeled $E^{(20)}$ corresponding to $\lambda = 0.001$, in Table I. That number is actually $3 + 4.091\lambda - 16\lambda^2$, where the first term is the unperturbed energy, the second is the first-order perturbation correction, Eq. (2.2), and the third is the contribution of all remaining nineteen states. The coefficient of λ^2 varies very slowly with the number of states of the basis: adding more figures, it changes from -14.97 for $N = 10$ to -16.16 for $N = 20$. Certainly, the energy eigenvalue decreases when increasing the number of basis states, but very slowly. This behavior is a direct consequence of the abnormal properties of the perturbation, as pointed out by Harrell in Ref. 1.

It is interesting to study this point more closely. Assume a very small λ and solve the matrix eigenvalue problem by expanding the determinant in powers of λ up to and including λ^2. As it is well known, we end up with the perturbation-like formula

$$E = E_0 + \langle 0|x^\beta|0\rangle\lambda - \lambda^2 \sum_{n\neq 0}^{N} \frac{|\langle 0|x^\beta|n\rangle|^2}{E_n - E_0},$$

(5.3)

with the difference that the sum in the λ^2 correction is limited to the chosen number of basis states. Analyzing this sum, we will understand the slow variation of the matrix eigenvalue problem solutions.

Using (3.13) for $\beta = -5/2$ there results

$$\sum_{n\neq 0} \frac{|\langle 0|x^\beta|n\rangle|^2}{E_n - E_0}$$
$$= \gamma \sum_{n\neq 0} \frac{1}{4n} \frac{(2+\frac{1}{2})^2}{2\cdot 3} \frac{(4+\frac{1}{2})^2}{4\cdot 5} \cdots \frac{(2n+\frac{1}{2})^2}{2n(2n+1)},$$

(5.4)

where $\gamma = \Gamma[(\beta + 3)/2]/\Gamma(3/2)$ and the factors $(2n + 1)!$ and $\beta(\beta - 2)\cdots(\beta - 2n + 2)$ have been ordered in a special form. The ratio of the $(n + 1)$th and nth terms of the sum in (5.4) is

$$\frac{\langle 0|x^\beta|n + 1\rangle^2/(E_{n+1} - E_0)}{\langle 0|x^\beta|n\rangle^2/(E_n - E_0)}$$

$$= \frac{n}{n + 1} \frac{(2n + 2 + \frac{1}{2})^2}{2(n + 1)(2n + 3)} \underset{n \to \infty}{\to} 1,$$

so that successive contributions to the coefficient of λ^2 are of the same size. Moreover, each of the grouped terms in (5.4) is bigger than 1, i.e.,

$$(2k + 1/2)/2k(2k + 1) > 1$$

and each term of (5.4), apart from a global constant, is bigger than the corresponding term of the harmonic series $\Sigma(1/n)$ which is known to be divergent.

Thus, the standard perturbation theory, Eq. (5.3) for $N \to \infty$, makes no sense, and our variational method will give a ground state energy which converges very slowly when the number of basis states increases. Note finally that Eq. (5.3) is no longer an upper bound formula, and it is only valid for N sufficiently small.

The variational results are somewhat poor for small λ and quite good for large λ. At small λ the non-power series expansion of Harrell[1] is appropriate, as well as at large λ our large coupling perturbation expansion gives a proper description of the ground state energy.

Finally we have the region of intermediate $\lambda(\simeq 1)$. In this region, the best method is the variational one. By using sufficiently large basis one could obtain the correct value of the energy, but no definite statements about the speed of the convergence can be drawn from our results.

In conclusion, it seems that the appropriate method to deal with this class of potentials is to use a nonpower series expansion for small coupling constant, and a large coupling perturbative expansion for large λ. Both expansions should be an appropriate extension of the presently known forms. Moreover, it would also be of interest to find a connection of both expansions for intermediate values of the coupling constant.

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APPENDIX

A program has been written in BASIC for symbolically handling the evaluation of the matrix elements of the operator x^β. A listing of the program can be obtained from the authors on request. The first ten matrix elements of x^β run as follows; where

$$x^\beta_{mn} \equiv \langle m - 1|x^\beta|n - 1\rangle,$$

$$x^\beta_{11} \equiv \gamma = \Gamma\left(\frac{\beta + 3}{2}\right)\Big/\Gamma(3/2),$$

$$x^\beta_{12} = \beta\gamma/\sqrt{3!},$$

$$x^\beta_{13} = \beta(\beta - 2)\gamma/\sqrt{5!},$$

$$x^\beta_{14} = \beta(\beta - 2)(\beta - 4)\gamma/\sqrt{7!},$$

$$x^\beta_{22} = (\beta^2 + 2\beta + 6)\gamma/3!,$$

$$x^\beta_{23} = \beta(\beta^2 + 2\beta + 12)\gamma/\sqrt{3!5!},$$

$$x^\beta_{24} = \beta(\beta^3 + 14\beta - 36)\gamma/\sqrt{3!7!},$$

$$x^\beta_{33} = (\beta^4 + 4\beta^3 + 36\beta^2 + 64\beta + 120)\gamma/5!,$$

$$x^\beta_{34} = \beta(\beta^4 + 4\beta^3 + 56\beta^2 + 104\beta + 360)\gamma/\sqrt{5!7!},$$

$$x^\beta_{44} = (\beta^6 + 6\beta^5 + 106\beta^4 + 454\beta^3$$
$$+ 1660\beta^2 + 3968\beta + 5040)\gamma/7!.$$

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