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Ground-state energy of singular potentials

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It is shown that for singular potentials of the form λ/r^α, the asymptotic form of the wave function both at $r \to \infty$ and $r \to 0$ plays an important role. Using a wave function having the correct asymptotic behavior for the potential λ/r^4, it is shown that it gives the exact ground-state energy for this potential when $\lambda \to 0$, as given earlier by Harrell [Ann. Phys. (NY) **105**, 379 (1977)]. For other values of the coupling parameter λ, a trial basis set of wave functions which also satisfy the correct boundary conditions at $r \to \infty$ and $r \to 0$ are used to find the ground-state energy of the singular potential λ/r^4. It is shown that the obtained eigenvalues are in excellent agreement with their exact ones for a very large range of λ values.

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I. INTRODUCTION

There is growing interest in the study of the harmonic oscillator to which a singular potential of the form λ/r^α is added [1–10]. There are several reasons for this interest. The first is that the ordinary perturbation theory badly fails for such singular potentials. The second is to find an approximate wave function which could be used over the entire region of λ. In the present work, we show that in choosing the approximate wave function, the asymptotic form both at $r \to \infty$ as well as $r \to 0$ plays an important role. The correct behavior of the eigenfunction in those limits is taken into account by means of a modified Gaussian function. We present the detailed calculations which we have carried out for the singular potential λ/r^4 and present the excellent results which are obtained for the ground-state energies for a large range of values of the coupling parameter λ.

We describe the essential formulation in Sec. II. A variational treatment is given in Sec. III. The numerical results are presented in Sec. IV, and concluding remarks are given in Sec. V.

II. FORMULATION

The Hamiltonian H is given by

$$H = -\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} + r^2 + \frac{\lambda}{r^4} \tag{1}$$

and defined in the space $L^2[0,\infty)$. It is obvious that for this Hamiltonian as $r \to \infty$, the term r^2 dominates while if $r \to 0$, the term $1/r^4$ dominates. The wave function which is appropriate for the behavior of the Hamiltonian given by (1) should therefore be of the form

$$R(r) = N \exp\left(-ar^2 - \frac{b}{r}\right), \tag{2}$$

N being the normalization constant and a, b being yet unknown parameters. This modified Gaussian dominates the behavior of any polynomial in r at infinity and vanishes at the origin. So, any function constructed as a product of a polynomial in r and $R(r)$ will still have the correct behavior at both limits. This fact will be useful in Sec. III, where we develop a variational calculation to get the eigenvalues (and the eigenfunctions) of the operator (1).

Putting the function (2) into the eigenvalue equation

$$HR = ER, \tag{3}$$

we find that the asymptotic forms at $r \to \infty$ and $r \to 0$ imply that

$$a = \frac{1}{2}, \quad b = \sqrt{\lambda}. \tag{4}$$

The ground-state energy E is then given by

$$E = 3 + 2\sqrt{\lambda}\frac{\int_0^\infty drr \exp\left(-r^2 - 2\sqrt{\lambda}/r\right)}{\int_0^\infty drr^2 \exp\left(-r^2 - 2\sqrt{\lambda}/r\right)}. \tag{5}$$

We now need to evaluate the integral of the form

$$I = \int_0^\infty drr^\beta \exp\left(-Ar^2 - \frac{B}{r}\right). \tag{6}$$

This integral can be evaluated as a series in Bessel functions K and confluent hypergeometric function M [11]. It is given by

$$I = \left[\frac{B}{A}\right]^{\frac{\beta+1}{3}} \left[\sum_{\nu=0}^{\infty} K_{\nu-(\beta+1)/2}[2(AB^2)^{1/3}] M\left(-\nu, \tfrac{1}{2}, -\tfrac{1}{4}(AB^2)^{1/3}\right) \frac{\left[(AB^2)^{1/3}\right]^{\nu}}{\nu!}\right.$$
$$\left. - \sum_{\nu=0}^{\infty} K_{\nu-\beta/2}[2(AB^2)^{1/3}] M\left(-\nu, \tfrac{3}{2}, -\tfrac{1}{4}(AB^2)^{1/3}\right) \frac{\left[(AB^2)^{1/3}\right]^{\nu+1}}{\nu!}\right]. \quad (7)$$

We shall now calculate the ground-state energy E given by expression (5) in the limit when $\lambda \to 0$. For this limit using the value of the Bessel function K when its argument goes to zero [11], we find that

$$E = 3 + \frac{4}{\sqrt{\pi}}\sqrt{\lambda}, \quad (8)$$

which is exactly the same value as given by Harrell [1].

It must be emphasized that an approximate wave function which does not satisfy the correct asymptotic form considerably over estimates this energy as has been noted recently by Fernández [4].

III. VARIATIONAL ANALYSIS

In this section, we develop a detailed variational analysis of the Hamiltonian (1). The variational function is taken as a linear combination of functions whose behaviors at $r \to 0$ *and* at $r \to \infty$ are determined by the modified Gaussian function introduced in Eq. (2), with a and b given by Eq. (4). Explicitly, the basis set of trial wave functions is given by

$$R_n(r) = A_n M\left(-n, \frac{3}{2}, r^2\right) \exp\left(-ar^2 - \frac{b}{r}\right), \quad (9)$$

where A_n is the normalization constant and $M(-n, 3/2, r^2)$ is the confluent hypergeometric function [11].

The basis set given by expression (9) is not orthogonal. We could have replaced M by new polynomials which are orthogonal with respect to the weight $\exp(-2ar^2 - 2b/r)$, but in the numerical work, it turns out to be simpler to use the wave functions given by (9) and calculate the overlap integrals to take into account the nonorthogonality of the wave functions. A diagonalization procedure adequate for the present situation is detailed in Sec. IV.

Let $I(u)$ be the integral given by

$$I(u) = \int_0^\infty r^u \exp\left(-r^2 - \frac{2\sqrt{\lambda}}{r}\right) dr, \quad (10)$$

which is of the form (6). The overlap integral $S_{mn} = \int_0^\infty R_m(r) R_n(r) r^2 dr$ is given in terms of $I(u)$ by

$$S_{mn} = A_m A_n \sum_{p=0}^{n} \sum_{q=0}^{m} \frac{\Gamma(p-n)\Gamma(3/2)}{\Gamma(-n)\Gamma(p+3/2)p!} \times \frac{\Gamma(q-m)\Gamma(3/2)}{\Gamma(-m)\Gamma(q+3/2)} \times I(2p+2q+2). \quad (11)$$

Instead of using the result shown in Eq. (7), for the present purpose it will be more convenient to use recursion relations for the integrals $I(u)$, discussed below.

We next give the expression for the Hamiltonian matrix element

$$H_{mn} = \langle R_m | H | R_n \rangle = \int_0^\infty R_m(r) H R_n(r) r^2 dr. \quad (12)$$

The expression for the matrix elements H_{mn} can be obtained by a direct calculation and is given by

$$H_{mn} = A_m A_n \sum_{p=0}^{n} \sum_{q=0}^{m} \frac{\Gamma(p-n)\Gamma(3/2)}{\Gamma(-n)\Gamma(p+3/2)p!} \frac{\Gamma(q-m)\Gamma(3/2)}{\Gamma(-m)\Gamma(q+3/2)q!} \times \left[(4m+3) I(2p+2q+4) + 2\sqrt{\lambda} I(2p+2q+1) - 4q\sqrt{\lambda} I(2p+2q-1)\right]. \quad (13)$$

This expression for the matrix elements H_{mn} can also be written in a form which shows the symmetric nature of the Hamiltonian by using partial integration.

The functions $I(u)$ can be calculated by numerically evaluating the integrals or by using the recursive relation

$$(u+1) I(u) = (u-1) I(u-2) + 2\sqrt{\lambda} I(u-3). \quad (14)$$

In the next section we describe the diagonalization of H in the nonorthogonal basis (9) and the final results for the ground-state energies.

IV. NUMERICAL RESULTS

In the following, we describe the procedure we used to diagonalize an Hermitian operator in a nonorthogonal basis. Let $\psi_i(r)$ and E_i be the exact eigenfunctions and eigenvalues of H. Then writing

$$\psi_i = \sum_j a_{ji} R_j(r), \quad (15)$$

the eigenvalue equation can be written as

TABLE I. Values of the ground-state energies calculated using the eigenvalue equation (18) for various values of λ. The subscript p in E_p denotes the dimension of the matrix. The "exact" values were obtained by numerically integrating the Schrödinger equation and were taken from Refs. [4] and [10]. (NA denotes not available.)

λ	E_1	E_2	E_4	E_6	E_8	E_{10}	Exact
0.001	3.06902	3.06884	3.06878	3.06877	3.06877	3.06877	NA
0.100	3.20698	3.20552	3.20517	3.20511	3.20509	3.20508	3.20507
0.100	3.58663	3.57730	3.57582	3.57564	3.57559	3.57557	3.57555
1.000	4.54139	4.49754	4.49443	4.49423	4.49419	4.49418	4.49418
10.000	6.75992	6.60824	6.60667	6.60663	6.60662	6.60662	6.60662
100.000	11.67745	11.26744	11.26508	11.26508	11.26508	11.26508	11.26508
1000.000	22.36324	21.43228	21.36946	21.36946	21.36946	21.36946	NA

$$Ha = SaE, \tag{16}$$

where a is the matrix formed by the eigenvector components a_{ij} and S is the overlap matrix.

Since S is a real symmetric matrix, it can be diagonalized by an orthogonal matrix P, i.e.,

$$PS\tilde{P} = d, \tag{17}$$

d_i being the eigenvalues of S.

Since all the d_i's turn out to be positive in the present problem, the eigenvalue equation can be rewritten as

$$(d^{-1/2}PH\tilde{P}d^{-1/2})(d^{1/2}Pa) = (d^{1/2}Pa)E, \tag{18}$$

and therefore the problem of finding the eigenvalues reduces to diagonalizing the real symmetric matrix $H' = d^{-1/2}PH\tilde{P}d^{-1/2}$. From the new eigenvector $\psi' = d^{1/2}Pa$ we could obtain the matrix a and, consequently, the eigenfunction (15) expressed in terms of the basis set defined in (9).

In order to get an idea of the trend of the method, the diagonalization was carried out in variational spaces of different dimensions. The final results for the ground-state energy are presented in Table I.

V. CONCLUDING REMARKS

In Table I, we have also given the exact values of the ground-state energies for various values of the coupling parameter λ. These values were obtained by Fernández [4] and Estévez *et al.* [10] through numerical integration of the corresponding Schrödinger equation. By examining the table, we find that the calculated values are in excellent agreement with the corresponding exact values for all values of λ. The convergence for both large and small values of the coupling parameter λ is remarkable. The convergence is also fast for intermediate values of λ.

Thus the present work establishes conclusively the result that not only the boundary condition at $r \to \infty$ plays an important role, but also the one at $r \to 0$. In other words, we have shown that the correct asymptotic form of the wave function $R(r)$ both when $r \to \infty$ as well as $r \to 0$ is essential in getting the exact ground-state energy for the singular potential λ/r^4.

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