

On the Exact Solution of the Schrödinger Equation with a Quartic Anharmonicity

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ABSTRACT

A new version of solutions in the form of an exponentially weighted power series is constructed for the two-dimensional circularly symmetric quartic oscillators, which reflects successfully the desired properties of the exact wave function. The regular series part is shown to be the solution of a transformed equation. The transformed equation is applicable to the one-dimensional problem as well. Moreover, the exact closed-form eigenfunctions of the harmonic oscillator can be reproduced as a special case of the present wave function. © 1996 John Wiley & Sons, Inc.

1. Introduction

The Schrödinger equation with the Hamiltonian of the form

$$H = -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + x^2 + y^2 + \beta(x^4 + 2a_{12}x^2y^2 + y^4), \quad \beta \geq 0 \quad (1.1)$$

is a simple, though nontrivial, quantum mechanical model which has been investigated very extensively in the last 25–30 years. Several methods, both analytical and numerical, have been developed to determine the energy eigenvalues E_{nl} and the eigenfunctions Ψ_{nl} of the eigenvalue problem:

$$H\Psi = E\Psi, \quad (1.2)$$

in which

$$\lim_{|r| \rightarrow \infty} \Psi(\mathbf{r}) = 0, \quad \mathbf{r} = (x, y). \quad (1.3)$$

There is, unfortunately, no exact solution which can be expressed as a finite combination of elementary functions except for the case of $\beta = 0$, where the potential simplifies into the harmonic oscillator $V(x, y) = x^2 + y^2$.

In this article, we deal mainly with the circularly symmetric oscillators when $a_{12} = 1$. If we let $x = r \cos \theta$ and $y = r \sin \theta$, the problem then turns out to be a separable one, and its radial part is found to be

$$\left(-\frac{d^2}{dr^2} - \frac{1}{r} \frac{d}{dr} + \frac{l^2}{r^2} + r^2 + \beta r^4 \right) R(r) = ER(r), \quad r \in [0, \infty) \quad (1.4)$$

for $l = 0, 1, \dots$. Now, the radial wave function $R(r)$ obeys the conditions

$$\lim_{r \rightarrow \infty} R(r) = 0, \quad \lim_{r \rightarrow 0} R(r) : \text{Finite.} \quad (1.5)$$

It is conventional to factor off the function r^l , i.e.,

$$R(r) = r^l \Phi(r), \quad (1.6)$$

where the differential equation satisfied by $\Phi(r)$ is

$$\begin{aligned} T\Phi &= E\Phi, \\ T &= -\frac{d^2}{dr^2} - \frac{2l+1}{r} \frac{d}{dr} + r^2 + \beta r^4, \\ r &\in [0, \infty). \end{aligned} \quad (1.7)$$

It is readily shown that for $\beta = 0$ Eq. (1.7) has exact solutions of the form

$$\Phi(r) = e^{-(1/2)r^2} \sum_{k=0}^n f_k r^{2k}, \quad n = 0, 1, \dots, \quad (1.8)$$

where

$$\begin{aligned} -(k+1)(k+l+1)f_{k+1} + (k-n)f_k &= 0, \\ k &= 0, 1, \dots, n-1 \end{aligned} \quad (1.9)$$

with eigenvalues

$$E \equiv E_{nl} = 2(2n+l+1), \quad n, l = 0, 1, \dots \quad (1.10)$$

The polynomial factor in (1.8) may be written in terms of associated Laguerre polynomials $L_n^{(l)}$ with argument r^2 .

We should note that the one-dimensional Schrödinger equation with a quartic anharmonicity

$$\begin{aligned} \left(-\frac{d^2}{dx^2} + x^2 + \beta x^4 - E \right) \Psi(x) &= 0, \\ x &\in (-\infty, \infty), \\ \lim_{|x| \rightarrow \infty} \Psi(x) &= 0 \end{aligned} \quad (1.11)$$

will also be considered here in connection with (1.7).

To provide a detailed historical perspective about the problem being considered is unnecessary. We indicate only a few properties and some of the major trends with their basic outlines. This system has a real positive spectrum which is discrete for each l fixed. Furthermore, two regimes of eigenvalues referred to as the "near harmonic" and "near pure anharmonic" may be distin-

guished depending on the anharmonicity constant β and the quantum number n .

A perturbation series solution to (1.2) can be shown to be divergent for all $\beta > 0$ [1-3]. Therefore, a perturbative treatment of the problem is valid only for the nearly harmonic regime. WKB-type analyses, on the other hand, give satisfactory results in the pure anharmonic regime [4-6]. In variational as well as in Hill's determinant methods, the wave function is generally expanded in terms of the scaled eigenfunctions of the harmonic oscillator [7-10]. Besides, there are, of course, several numerical procedures to solve eigenvalue problems of this kind [11-17].

The Hill-Taylor approach to the construction of series solutions used the correct asymptotic behavior of the wave function as a weighting factor [15, 18]. In general, the behavior of a physical system modeled by a differential equation is most interesting in the vicinity of singular points. Actually, singular points determine the principal features of the solution to a large extent. Equations (1.7) and (1.11) have irregular singularity at infinity. An extra regular singular point of the radial Schrödinger equation is located at the origin, which has already been taken care of by the factor r^l in (1.6). So, it is useful to examine the asymptotic behavior of the wave function for very large values of r . The leading order asymptotic solution of $T\Phi = E\Phi$, which vanishes as $r \rightarrow \infty$, is

$$\Phi(r) \approx e^{-(1/3)\sqrt{\beta}r^3}. \quad (1.12)$$

After substitution of this into the equation, we see that

$$\frac{T\Phi(r)}{\Phi(r)} = O(r^2), \quad r \rightarrow \infty. \quad (1.13)$$

To be more accurate, the next-order correction is taken into account by writing

$$\Phi(r) \approx e^{-(1/3)\sqrt{\beta}r^3 - (1/2\sqrt{\beta})r}, \quad (1.14)$$

which makes the ratio $T\Phi/\Phi$,

$$\frac{T\Phi(r)}{\Phi(r)} = O(r), \quad (1.15)$$

as $r \rightarrow \infty$. Even the last form which is introduced in Hill-Taylor approach is not enough, because

the ratio $T\Phi/\Phi$ does not lead to E as $r \rightarrow \infty$. The linearity of T implies immediately, from (1.7), that

$$T^k\Phi = E^k\Phi, \quad T^0 \equiv 1, \quad k = 0, 1, \dots \quad (1.16)$$

and that $T\Phi/\Phi, T^2\Phi/\Phi, \dots$ are all bounded. Therefore, the desired asymptotic solution should be taken in the form

$$\Phi(r) \approx e^{-(1/3)\sqrt{\beta}r^3 - (1/2\sqrt{\beta})r - (1/2)(2l+3)\ln r}, \quad (1.17)$$

for which the ratio

$$\frac{T\Phi(r)}{\Phi(r)} = O(1) \quad (1.18)$$

is bounded as $r \rightarrow \infty$. Now, it is not difficult to show that $T^2\Phi/\Phi, T^3\Phi/\Phi, \dots$ are also bounded as $r \rightarrow \infty$. Hence, a full solution in the form of power series weighted by (1.17) may be proposed. The series part of such a candidate solution is expected to be regular for all r including infinity.

One more obvious fact is that if we had the exact solution at hand we would derive continuously the closed-form eigenfunctions given in (1.8) as β approaches zero. However, the exponential factor in the above-mentioned candidate solution can never turn out to be $e^{-(1/2)r^2}$ as $\beta \rightarrow 0$ in a like manner. This simple heuristic argument suggests evidently that there is still something missing.

Moreover, in the one-dimensional case, we are confronted with an additional complication due to the appearance of an absolute value function in the leading term of the asymptotic solution. Clearly, Eq. (1.11) has solutions of the form

$$\Psi(x) \approx \begin{cases} e^{-(1/3)\sqrt{\beta}x^3}, & x > 0 \\ e^{(1/3)\sqrt{\beta}x^3}, & x < 0 \end{cases} \quad (1.19)$$

for sufficiently large values of $|x|$ satisfying the boundary conditions at infinity. As a result, if we look for solutions in this way, it would be necessary to match the two eigenfunctions valid for $x > 0$ and $x < 0$, respectively, at $x = 0$.

In the following text, an appropriate coordinate transformation of the independent variable is proposed that clears up the difficulties pointed out above. We then determine the exponential part by taking into consideration not only the asymptotic behavior of the wave function, but also the requirement that $T\Phi/\Phi$ has to be bounded as $r \rightarrow \infty$. Finally, it is shown that the eigenvalues of the problem may be computed to any desired accuracy by converging Hill's determinant procedure.

2. The Transformed Problem

Instead of (1.7), it is more convenient to consider the rescaled equation of the form

$$\left[-\frac{d^2}{dr^2} - \frac{2l+1}{r} \frac{d}{dr} + \nu^2 r^2 + (1-\nu^3)r^4 \right] \times \Phi(r) = \nu E \Phi(r), \quad (2.1)$$

in which the parameter ν is defined by

$$\nu = (1 + \beta)^{-1/3} \quad (2.2)$$

in terms of the original coupling constant β . The new system parameter ν lies between $1 \geq \nu \geq 0$ as β varies from zero to infinity. The discussion in the first section motivates the introduction of the following coordinate transformation: If we change the independent variable from r to ξ ,

$$\xi = (1 + \alpha r^2)^{-1/2}, \quad 0 < \alpha < \infty, \quad (2.3)$$

the "point at infinity" is taken into the origin on the ξ -axis. We hope that the nonnegative parameter α will help somehow to extract the exact harmonic eigensolutions.

The Schrödinger Eq. (2.1) then becomes

$$\tilde{T}\Phi(\xi) = \nu E \Phi(\xi), \quad \xi \in [0, 1], \quad \Phi(0) = 0, \quad (2.4)$$

where the transformed Hamiltonian \tilde{T} is of the form

$$\tilde{T} = \alpha \xi^4 (\xi^2 - 1) \frac{d^2}{d\xi^2} + \alpha \xi^3 (3\xi^2 + 2l - 1) \frac{d}{d\xi} + \frac{\nu^2}{\alpha} \left(\frac{1}{\xi^2} - 1 \right) + \frac{1 - \nu^3}{\alpha^2} \left(\frac{1}{\xi^2} - 1 \right)^2. \quad (2.5)$$

From the aforementioned considerations, the wave function should contain an exponential factor,

$$\begin{aligned} \Phi(\xi) &\approx e^{g(\xi)}, \\ g(\xi) &= -\frac{1}{3}a\xi^{-3} + b\xi^{-1} + c \ln \xi, \\ a &> 0, \end{aligned} \quad (2.6)$$

because of the irregular singularity located at $\xi = 0$. Substituting (2.6) into (2.4), we have, for small ξ , the result

$$\begin{aligned} \tilde{T}\Phi &\approx \alpha^{-2} \{ (1 - \nu^3 - \alpha^3 a^2) \xi^{-4} \\ &+ [2\alpha^3 ab + \alpha^3 a^2 - 2(1 - \nu^3) + \alpha \nu^2] \xi^{-2} \\ &+ \alpha^3 a(2l + 3 - 2c) \xi^{-1} + O(1) \} \Phi, \end{aligned} \quad (2.7)$$

which shows that $\tilde{T}\Phi/\Phi$ remains finite at $\xi = 0$, if

$$2c = 2l + 3 \tag{2.8}$$

$$2\alpha^3 ab + \alpha^3 a^2 - 2(1 - \nu^3) + \alpha\nu^2 = 0 \tag{2.9}$$

$$1 - \nu^3 - \alpha^3 a^2 = 0. \tag{2.10}$$

The function (2.6) can be rewritten as

$$\Phi(\xi) \approx \xi^c e^{-(1/3)a\xi^{-3} + b\xi^{-1}}, \tag{2.11}$$

with a and b being dependent upon α , and c defined by (2.8). From (2.10), we see that α tends to zero when ν is equal to 1. But the case of $\nu = 1$ corresponds to a harmonic oscillator problem whose wave function contains the well-known exponential factor $e^{-(1/2)r^2}$. We may, therefore, argue that $-\frac{1}{3}\xi^{-3} + b\xi^{-1}$ in (2.11) should converge to $-\frac{1}{2}r^2$ as $\alpha \rightarrow 0^+$. Thus, we must have

$$\lim_{\alpha \rightarrow 0^+} \left[-\frac{1}{3}a(1 + \alpha r^2)^{3/2} + b(1 + \alpha r^2)^{1/2} \right] = -\frac{1}{2}r^2, \tag{2.12}$$

from which it follows that

$$\lim_{\alpha \rightarrow 0^+} \left[-\frac{1}{3}a\left(1 + \frac{3}{2}\alpha r^2 + \frac{3}{8}\alpha^2 r^4 + \dots\right) + b\left(1 + \frac{1}{2}\alpha r^2 - \frac{1}{8}\alpha^2 r^4 + \dots\right) \right] = -\frac{1}{2}r^2 \tag{2.13}$$

and that

$$\alpha(a - b) = 1. \tag{2.14}$$

Obviously, the constant term $-\frac{1}{3}a + b$ on the left-hand side of (2.13) is unimportant since it changes only the proportionality constant implicitly defined in (2.11). Hence, the mathematically elegant formula for α ,

$$\alpha = (1 - \nu^3) \left[1 + (1 - \nu^2)^{1/2} \right]^{-2}, \tag{2.15}$$

is obtained, being a smooth bounded function of ν . Note that absolute extremum values of α calculated at $\nu = 1$ and $\nu = 0$ are, respectively, 0 and $\frac{1}{4}$. Finally, the determination of the other parameters can be accomplished by the relations

$$a = (1 - \nu^3)^{1/2} \alpha^{-3/2} \tag{2.16}$$

and

$$b = (1 - \nu^2)^{1/2} \alpha^{-1}. \tag{2.17}$$

If we now look at the rescaled one-dimensional quartic oscillator

$$\left[-\frac{d^2}{dx^2} + \nu^2 x^2 + (1 - \nu^3)x^4 \right] \Psi(x) = \nu E \Psi(x), \quad x \in (-\infty, \infty) \tag{2.18}$$

in the same picture, we can make use of the similar mapping

$$\xi = (1 + \alpha x^2)^{-1/2}, \quad \xi \in [0, 1] \tag{2.19}$$

which is no longer one-to-one. However, using the fact that the wave function is either symmetric or antisymmetric, there is no complication in returning back to the original variable x . Furthermore, we observe that the treatment of the problem is completely unaltered in form provided that $c = 1$. Therefore, omitting expression (2.8) for c and letting $c = 1$ enables the independent treatment of the one-dimensional case in this context, without any modification. It should be noticed merely that the role of the transformation (2.19), here, is twofold. First, it removes the absolute value function appearing in the asymptotic solution (1.19). Thus, a matching procedure is not needed anymore. Second, by means of (2.14), the exponential factor approaches the harmonic oscillator weighting function $e^{-(1/2)x^2}$ as $\nu \rightarrow 1$, as in the two-dimensional case.

This kind of analysis consequently suggests the proposition of the exact wave function in the form

$$\Phi(\xi) = \xi^c e^{-(1/3)a\xi^{-3} + b\xi^{-1}} F(\xi). \tag{2.20}$$

It is clear that the required vanishing behavior of $\Phi(\xi)$ at the origin of the transformed domain is fulfilled if $F(\xi)$ grows no faster than $e^{(1/3)a\xi^{-3}}$ as $\xi \rightarrow 0^+$. Transforming the dependent variable from $\Phi(\xi)$ to $F(\xi)$, it is shown that $F(\xi)$ satisfies the differential equation

$$(\mathcal{L} - \nu E)F(\xi) = 0, \quad \xi \in (0, 1], \tag{2.21}$$

where the operator \mathcal{L} is defined by

$$\begin{aligned} \mathcal{L} = & \alpha \xi^4 (\xi^2 - 1) \frac{d^2}{d\xi^2} + \alpha [(2c + 3)\xi^5 \\ & + 2b\xi^4 - 4\xi^3 + 2(a + b)\xi^2 - 2a] \frac{d}{d\xi} \\ & + \alpha \{c(c + 2)\xi^4 - b(2c + 1)\xi^3 \\ & + (b^2 + c^2 - 3c)\xi^2 \\ & + [a(2c - 1) + 2b]\xi - b^2\}. \end{aligned} \tag{2.22}$$

Since the resulting eigenvalue equation admits a regular solution for $F(\xi)$ which remains finite for all sufficiently small positive ξ , the wave function in (2.20) really satisfies the boundary condition. This will be justified properly in Section 4.

Equation (2.21) has regular singular points at $\xi = \mp 1$ apart from the essential singularity at the origin, in the ξ -complex plane. The point $\xi = -1$ is, however, out of the interval of interest. According to the basic theory of differential equations, a series expansion of $F(\xi)$ about the point $\xi = 1$ is sure to exist with a unit radius of convergence. Such a solution is, therefore, valid in the whole physical domain of ξ and vanishes at $\xi = 0$ when it is multiplied by the function in (2.11).

3. The Series Solution

Owing to the regular singularity of the point $\xi = 1$, it is natural to seek solutions for (2.21) of the form

$$F(\xi) = \left[\frac{2}{\alpha}(1 - \xi) \right]^{\rho} \sum_{n=0}^{\infty} \left(-\frac{2}{\alpha} \right)^n f_n (\xi - 1)^n, \quad (3.1)$$

where the factor $(-2/\alpha)^n$ in the coefficients of the series has been introduced for convenience. Substituting (3.1) into the eigenvalue equation, shifting indices of summations, and equating coefficients of like powers of $(\xi - 1)$ to zero yield

$$\rho(2\rho + 2c - 3) = 0 \quad (3.2)$$

and

$$\begin{aligned} & -(2n + 2\rho + 2c - 1)(2n + 2\rho + 2)f_{n+1} \\ & + (9\alpha(n + \rho)(n + \rho - 1) \\ & + [5(2c + 3)\alpha - 12\alpha + 4](n + \rho) \\ & + (2c - 1)(1 + \alpha c) - \nu E)f_n \\ & - \frac{1}{2}\alpha^2\{16(n + \rho - 1)(n + \rho - 2) \\ & + 2[\alpha - 5b + 5(2c + 3) - 6](n + \rho - 1) \\ & + (2c - 1)a - (6c + 1)b + 2b^2 \\ & + 2c(3c + 1)\}f_{n-1} \\ & + \frac{1}{4}\alpha^3\{14(n + \rho - 2)(n + \rho - 3) \\ & + 2[5(2c + 3) - 4b - 2](n + \rho - 2) \\ & + b^2 - 3(2c + 1)b + c(7c + 9)\}f_{n-2} \end{aligned}$$

$$\begin{aligned} & - \frac{1}{8}\alpha^4\{6(n + \rho - 3)(n + \rho - 4) \\ & + [5(2c + 3) - 2b](n + \rho - 3) \\ & + 4c(c + 2) - (2c + 1)b\}f_{n-3} \\ & + \frac{1}{16}\alpha^5\{(n + \rho - 4)(n + \rho - 5) \\ & + (2c + 3)(n + \rho - 4) \\ & + c(c + 2)\}f_{n-4} = 0, \quad (3.3) \end{aligned}$$

with $n = 0, 1, \dots$, where $f_{-4} \equiv \dots \equiv f_{-1} \equiv 0$.

Equation (3.2) is the so-called indicial equation whose roots $\rho_1 = 0$ and $\rho_2 = \frac{3}{2} - c$ are the exponents of the singularity at $\xi = 1$. For the two-dimensional oscillator, however, the second root ρ_2 leads to a series solution containing most likely a logarithmic term, which is to be rejected since it does not satisfy the regularity condition at $\xi = 1$, or, originally, at $r = 0$. On the contrary, in the one-dimensional case where $c = 1$, both roots $\rho_1 = 0$ and $\rho_2 = \frac{1}{2}$ make sense, representing, respectively, the even and the odd eigenfunctions due to the fully symmetric structure of the starting potential $V(x) = x^2 + \beta x^4$.

From the fifth-order difference Schrödinger Eq. (3.3), we determine the coefficients f_n of the series solutions corresponding to each admissible energy E . Linear combination constants of those solutions can then be evaluated from the usual normalization condition.

By means of the definition of a truncated solution,

$$F(N; \xi) = \left[\frac{2}{\alpha}(1 - \xi) \right]^{\rho} \sum_{n=0}^{N-1} \left(-\frac{2}{\alpha} \right)^n f_n (\xi - 1)^n, \quad (3.4)$$

the infinite series (3.1) can be split into two parts:

$$F(\xi) = F(N; \xi) + S(N; \xi), \quad (3.5)$$

where the remainder $S(N; \xi)$ vanishes for sufficiently large values of N , since $F(\xi)$ is convergent in $\xi \in (0, 1]$. Now if we replace the problem (2.21) by the truncated one,

$$[\mathcal{L} - \nu E(N)]F(N; \xi) = 0, \quad (3.6)$$

it is easily seen that the substitution of (3.5) into (2.21) gives the relation

$$\nu[E - E(N)]F(N; \xi) = (\mathcal{L} - \nu E)S(N; \xi), \quad (3.7)$$

and, hence, we obtain, formally, that

$$\lim_{N \rightarrow \infty} E(N) = E. \quad (3.8)$$

In the truncated problem, the linear recurrences (3.3) may be regarded a homogeneous system of algebraic equations of order N . The coefficient matrix, $\Delta(E)$ say, of this system is of a banded Hessenberg form. Consequently, the roots of its characteristic equation are identified with truncated eigenvalues $E(N)$. Therefore, we may calculate the spectrum to any desired accuracy by systematically increasing the size N of the truncation. Certain specimen numerical results are presented in Tables I–V for the sake of illustration.

4. Justification of the Procedure

In his valuable article on Hill's determinant method, Hautot [19] discussed the vanishing condition of $\det \Delta(E) = 0$. As was clearly stated there, this condition, which is based on one of the basic theorems of linear algebra about homogeneous systems of a finite number of equations, is not necessarily true when the system being considered is an infinite one. In fact, the condition $\det \Delta(E) = 0$ is also closely related to the square integrability of the resulting wave function. Here, we deduce that our wave function in (2.20) and (3.4) describes the physical phenomena in connection with the vanishing of Hill's determinant.

As an explanatory guide, we first consider the one-dimensional harmonic oscillator

$$-\Psi''(x) + (x^2 - E)\Psi(x) = 0, \\ \Psi(x) = 0 \text{ as } |x| \rightarrow \infty. \quad (4.1)$$

Writing

$$\Psi(x) = e^{-(1/2)x^2} y(x) \quad (4.2)$$

and showing that $y(x)$ satisfies the transformed equation, namely, Hermite's differential equation

$$y'' - 2xy' + (E - 1)y = 0, \quad (4.3)$$

we then suppose a solution in the form

$$y(x) = \sum_{n=0}^{\infty} a_n x^{2(n+\rho)}, \quad (4.4)$$

where $\rho = 0$ and $\frac{1}{2}$, i.e., even and odd states, respectively. Now the wave function (4.2) is a physical solution if $y(x)$ does not grow faster than $e^{(1/2)x^2}$ as $|x| \rightarrow \infty$. For large enough values of x , Hermite's differential equation has solutions of the form

$$y(x) \approx e^{Ax^2} \quad (4.5)$$

upon substitution of which into (4.3) gives

$$[4A(A - 1)x^2 + 2A + E - 1]e^{Ax^2} = 0. \quad (4.6)$$

The last equation implies the two asymptotic solutions

$$y_1(x) \approx \text{Constant}, \quad y_2(x) \approx e^{x^2}, \quad (4.7)$$

corresponding to $A = 0$ and $A = 1$, respectively. Therefore, if $y(x)$ in (4.4) converges to $y_1(x)$ as $x \rightarrow \infty$, up to an unimportant factor, $\Psi(x)$ is then the desired solution. To ensure this, however, we take $E = 1$ as the ground-state energy, making $y(x)$ exactly a constant and the corresponding exact eigenfunction. In this way, we furnish the full spectrum of the harmonic oscillator.

TABLE I
The ground and the first excited states eigenvalues of the one-dimensional oscillator as a function of β .

β^a	N	E_0 (for $\rho_1 = 0$)	N	E_1 (for $\rho_2 = \frac{1}{2}$)
0	—	1	—	3
0.00001	3	1.000007499868755	4	3.000037498968811
0.1	12	1.065285509543718	14	3.306872013152914
1000	18	1.063978871132805	21	3.808683345938226
∞	2.0	1.060362090484183	21	3.799673029801394

^a Eigenvalues are equal to $\beta^{-1/3}E_n$ for $\beta > 1$.

TABLE II
Ground-state eigenvalues E_{00} as a function of β .

β^a	N	E_{00}
0	—	2
0.00001	4	2.000019999550022
1	20	2.952050091962874
1000	21	2.351338918312985
100,000	21	2.345131451302559
∞	22	2.344829072744275

^a Eigenvalues are equal to $\beta^{-1/3}E_{00}$ for $\beta > 1$.

In the present study, the transformed Eq. (2.21) plays the same role with Hermite's differential equation. Similarly, it may be shown by direct substitution that the two asymptotics of (2.21) are

$$F_1(\xi) \approx \text{Bounded}, \quad F_2(\xi) \approx e^{(2/3)\alpha\xi^{-3} - 2b\xi^{-1}} \quad (4.8)$$

as $\xi \rightarrow 0^+$. Without giving a rigorous proof, it is not a surprise that after having solved the difference Eqs. (3.3) in the asymptotic domain of $n \gg 1$ we get estimates leading to both $F_1(\xi)$ and $F_2(\xi)$ for sufficiently small positive values of ξ . As a consequence, if $F(\xi)$ behaves correctly at the origin, like $F_1(\xi)$, the wave function (2.20) then vanishes at $\xi = 0$. More specifically, from (3.5), we may write

$$\lim_{\xi \rightarrow 0^+} F(\xi) = M(N) + \sum_{n=N}^{\infty} \left(\frac{2}{\alpha}\right)^n f_n, \quad (4.9)$$

where $M(N)$ is a finite number. To avoid the unphysical situation of $F_2(\xi)$, we enforce $F(\xi)$ to remain bounded at $\xi = 0$ assuming that

$$f_N \equiv f_{N+1} \equiv \dots \equiv 0, \quad (4.10)$$

which is completely equivalent to equating Hill's determinant to zero. Therefore, in our case, the condition of $\det \Delta(E) = 0$ includes the requirement of square integrability of the wave function. Furthermore, it justifies our proposal of considering truncated solutions.

From a numerical point of view, on the other hand, (4.10) allows us a backward calculation of the coefficients f_n . This is important since the forward recursion in (3.3) spontaneously computes the dominant unbounded solution generated by $F_2(\xi)$, whereas the backward recursion is suitable for the stable computation of the bounded solution required [20].

5. Conclusion

In this article, a series representation of the exact solution of an old problem of quantum mechanics has been determined. The treatment is elementary so that further comments on the method itself are unnecessary. However, it may be interesting to examine particular cases.

For $\beta = 0$, or equivalently $\nu = 1$ where α is equal to zero from (2.15), we have the harmonic oscillator problem. In the one-dimensional case, the new variable ξ may be written as

$$\xi = 1 - \frac{1}{2}\alpha x^2 + O(\alpha^2), \quad \alpha \rightarrow 0^+ \quad (5.1)$$

and the solution (3.1) of the transformed equation becomes

$$F(x) = x^{2\rho} \sum_{n=0}^{\infty} f_n x^{2n} \quad (5.2)$$

in terms of the original variable x , when $\alpha = 0$.

TABLE III
The first and the second excited state eigenvalues as a function of β , when $l = 0$.

β^a	N	E_{10}	N	E_{20}
0	—	6	—	10
0.00001	5	6.000139993550605	6	10.00037997225402
1	22	10.88243555768198	25	20.66108269059789
1000	25	9.543744980405963	28	18.75490371420265
100,000	25	9.530429716668896	29	18.73611048361941
∞	25	9.529781384014808	29	18.73519550470177

^a Eigenvalues are equal to $\beta^{-1/3}E_{n0}$ for $\beta > 1$.

TABLE IV
First three eigenvalues as a function of β , where $l = 1$.

β^a	E_{01}	E_{11}	E_{21}
0	4	8	12
0.00001	4.000059998050135	8.000239985901665	12.00053995335796
1	6.462905999863872	15.48277157725167	25.96916356856702
1000	5.405485579551944	13.82830384294424	23.79818784259574
100,000	5.394750010063956	13.81190784608358	23.77682865174465
∞	5.394227164172288	13.81110953687373	23.77578876640046

^a Eigenvalues are equal to $\beta^{-1/3}E_{n1}$ for $\beta > 1$.

The recurrence relation (3.3) then reduces to

$$-(2n + 2\rho + 1)(2n + 2\rho + 2)f_{n+1} + [4(n + \rho) + 1 - E]f_n = 0, \quad n = 0, 1, \dots, \quad (5.3)$$

which implies that the series in (5.2) can be terminated at $n = k$ so as to give Hermite polynomials of order $2(k + \rho)$ [21], if

$$E = E_k = 4(k + \rho) + 1, \quad k = 0, 1, \dots \quad (5.4)$$

The last equation is the exact expression of the symmetric and antisymmetric harmonic eigenvalues corresponding to $\rho_1 = 0$ and $\rho_2 = \frac{1}{2}$, respectively.

Conversely, the use of (5.1) shows that the transformed Eq. (2.21) itself returns to Hermite's differential equation as α tends to zero. In entirely the same way, we can obtain the harmonic eigen-solutions given in (1.8) and (1.10), for the two-dimensional problem. Thus, the well-known exact solution of the harmonic oscillator can be reproduced from the present solution as its limiting case for $\alpha = 0$.

Another extreme case, the infinite-field limit Hamiltonian, corresponds to $\beta \rightarrow \infty$, or $\nu = 0$. Now, Eq. (2.1) takes the form

$$\left(-\frac{d^2}{dr^2} - \frac{2l + 1}{r} \frac{d}{dr} + r^4 \right) \Phi(r) = \mathcal{E} \Phi(r), \quad (5.5)$$

which is called the pure quartic oscillator. Here, the eigenvalue parameter \mathcal{E} is connected with the energy eigenvalues by the relation

$$E = \beta^{1/3} \mathcal{E}. \quad (5.6)$$

This is the usual asymptotic relation showing that the total energy of the system grows like $\beta^{1/3}$ as $\beta \rightarrow \infty$. For this extreme case of $\nu = 0$, we may get the solution without any trouble where the parameters α , a , and b have the following values:

$$\alpha = \frac{1}{4}, \quad a = 8, \quad b = 4. \quad (5.7)$$

Numerical evaluations for $\beta \rightarrow \infty$ are given in the last rows of the Tables I-V in terms of the eigenvalue parameter \mathcal{E} . We see from the tables that there is no accuracy loss for this limiting case of β . In the tables, the eigenvalues for $\beta > 1$ are replaced by $\beta^{-1/3}E$ to show how rapidly they converge to the $\beta \rightarrow \infty$ limit.

TABLE V
First three eigenvalues as a function of β , when $l = 2$.

β^a	E_{02}	E_{12}	E_{22}
0	6	10	14
0.00001	6.000119994900454	10.00035997450361	14.00071992861397
1	10.39062729550378	20.29382970753589	31.42392978589736
1000	8.943343403374937	18.33063381077860	28.98790098571932
100,000	8.928790864870353	18.31121872013153	28.96396281974264
∞	8.928082199849951	18.31027343240361	28.96279738893391

^a Eigenvalues are equal to $\beta^{-1/3}E_{n2}$ for $\beta > 1$.

In each table, various eigenvalues accurate to 16 digits are reported. We present the first two eigenvalues E_n of the one-dimensional quartic oscillator for some typical values of the coupling constant β including zero and infinity in Table I. Eigenvalues of higher-excited states were calculated within an excellent accuracy. However, the results are not quoted here since such tabulated data can be found in the literature, especially, in [8] and [15].

For the two-dimensional Schrödinger equation, the trivial eigenvalue ordering properties

$$E_{n+1,l} > E_{n,l} \quad (5.8)$$

and

$$E_{n,l_2} > E_{n,l_1}, \quad l_2 > l_1 \quad (5.9)$$

can be deduced from the Tables II–V. Tables I–III also include the truncated size N for which the converged eigenvalues are obtained. It is shown that the rate of convergence for the one-dimensional and the two-dimensional cases is more or less the same. We note that the eigenvalues E_{nl} of the circularly symmetric two-dimensional oscillators with such an accuracy are reported for the first time. Furthermore, the accuracy of our method is not limited by 16 significant figures. Actually, the accuracy of the eigenvalues may be improved arbitrarily depending on the machine accuracy of the computer. Here, we have never used a truncation size N , which is greater than 30, for the calculation of E_{nl} with $n, l = 0, 1, 2$. The results are in good agreement with previously published data [6, 8, 12, 15].

It is straightforward to extend the present solution for two-mode problem to N -mode oscillators. Another remark is that our main goal is to solve a more general problem, for instance, the Schrödinger equation with the potential

$$V(x, y) = w_1 x^2 + w_2 y^2 + \beta(a_{11} x^4 + 2a_{12} x^2 y^2 + a_{22} y^4). \quad (5.10)$$

We observed that the treatment of the circularly symmetric case along this line provides an impor-

tant background to this end. Further studies on more interesting problems are in progress, and they will be reported in due course.

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