Asymptotic series for wave functions and energy levels of doubly anharmonic oscillators

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Asymptotic series expansions for the wave functions and energy levels of the doubly anharmonic-oscillator system of the $ax^2+bx^4+cx^6$ type have been obtained. The asymptotic expansion for the wave function reduces to a sequence of exact solutions of the Schrödinger equation for special values of certain combinations of the coupling constants. A WKB-type analysis for large values of n (the excitation quantum number) yields an asymptotic expression for the excited energy levels, valid for large values of the dominant coupling. Exact eigenvalues have been computed numerically for a wide range of n and c, the dominant coupling. The accuracy of the asymptotic series for the energy eigenvalues of excited states is examined by comparison with the exact eigenvalues obtained numerically and is found to be satisfactory.

I. INTRODUCTION

The quantum mechanics of the anharmonic oscillator has been the subject of numerous investigations. Apart from providing a simple model for field theories with polynomial interactions, it is a system with considerable intrinsic interest. As a simple system which is not (yet) exactly soluble, its study has led to the development of analytic and approximation methods of wider applicability. Thus while in quantum electrodynamics it has only been conjectured that the perturbation series is of an asymptotic nature, Simon[1] rigorously proved that the Rayleigh-Schrödinger perturbation series for the energy eigenvalues of the anharmonic oscillator, while divergent for all values of the major coupling λ, is an asymptotic one in an open domain around $\lambda=0$. Again, while Bender and Wu[2] showed how WKB techniques may be used to study the analytic properties of the energy eigenvalues in the complex λ plane, Simon used Hilbert-space methods to obtain this analytic structure rigorously.

A wide variety of nonperturbative approximation schemes have been used to study the energy eigenvalues. Among these are numerical analyses using Padé approximants,[3] truncated Hill determinants in nonorthogonal basis,[4,5] and Bargmann space representations.[6-8] The numerical methods are often tedious when applied to the region where λ or n (or both) is large; hence there have been attempts to obtain approximate formulas for the eigenvalues in this region. Classical periodic solutions used in conjuction with the WKB method yield approximate formulas for large λ.[9-11] Asymptotic expressions for the energy eigenvalues valid in the large (λ, n) regime have been obtained[6-8] using modified WKB techniques. Surprisingly, the expressions obtained are accurate even for n as small as 3 and $\lambda > 2$.

Anharmonic systems of greater complexity have also been investigated recently.[12] Interacting quartic oscillators of the type $\lambda_1 x_1^4+\lambda_2 x_2^4+\lambda x_1^2 x_2^2$ have been studied by Hioe.[13] Numerical algorithms used for quartic oscillators have been extended to this interacting system.[8] While the rate of convergence for the energy eigenvalues is distinctly slower, the study reveals a level crossing pattern of considerable complexity. Doubly anharmonic systems of the type $ax^2+bx^4+cx^6$ have been studied analytically.[14-19] The eigenvalue problem can be reduced to the solution of a three-term difference equation with contiguous terms. This allows an analytic study of the Green's function of the system in a manner not possible for λx^{2m} oscillators. Examined in this fashion, this system has structural similarities with certain "confined" two-particle systems. The Schrödinger equation for a nonrelativistic two-particle system interacting through a confinement potential with terms depending on r^2 r, $1/r$, and $1/r^2$ (r being the magnitude of the relative two-particle separation) can be reduced to a similar three-term difference equation.[20] Such is also the case for a rotating spherical oscillator whose energy levels and wave functions in the asymptotic domain have been investigated.[21,22] This suggests that the study of the wave functions and energy levels of the doubly anharmonic system may, apart from any intrinsic interest, shed light on the behavior of other physical systems.

In this paper, we study analytically the wave functions and excited energy levels of doubly anharmonic oscillators of the type $ax^2+bx^4+cx^6$ in the asymptotic domain. In Sec. II, we use a WKB-type ansatz to examine the eigenvalue equation in the large-x region. We are thus able to obtain the leading oscillatory behavior of the wave function in this region. Factoring out this behavior, we obtain the asymptotic series for the wave function in this domain and the recursion relation for the coefficients. From the solution of this recursion relation, we can obtain a sequence of exact solutions for special values of certain combinations of the coupling constants. To examine the energy levels, we use a modified WKB method originally developed by Titchmarsh[23] for the study of a class of eigenvalue problems. This has been applied to the λx^4 case by Hioe, MacMillen, and Montroll.[6-8] In Sec. III we show that in spite of the presence of a subdominant coupling, the asymptotic series for the energy eigenvalues of the excited states, valid for large values of the dominant coupling, may be obtained by the same methods. Further, the series reduces to that for the λx^6 oscillator in the limit in which b, the subdominant coupling, vanishes. In Sec. IV we examine the accuracy of this asymptotic series by computing numerically the exact eigenvalues corresponding to the excited states of the oscillator and comparing them with the result obtained by using the first four terms of the asymptotic series. We compute the exact eigenvalues for a wide range of values of the excitation number n ($1 \leq n \leq 100$) and the major coupling c ($1 \leq c \leq 100$) using the method of truncated Hill determinants modified by the use of scaled basis functions. In general, the accuracy of the series increases with the magnitude of both c and n. We also examine the situation which obtains for negative values of the subdominant coupling b. We find the accuracy of the series comparable to the earlier case ($b > 0$) provided $c \geq |b|$; in both cases ($b \gtrless 0$) the accuracy of the series is comparable to that for the simpler λx^6 oscillator ($b = 0$).

II. THE WAVE FUNCTION IN THE ASYMPTOTIC DOMAIN: EXACT SOLUTIONS

We write the Schrödinger equation for the doubly anharmonic oscillator in the form

$$\frac{-d^2\psi}{dx^2} + (ax^2 + bx^4 + cx^6 - E)\psi = 0 \qquad (1)$$

(in units $\hbar = 2m = 1$). The couplings a, b, c are real; a and $c > 0$. The construction of the wave function for $x \to \infty$ starts with the identification that $x = \infty$ is an irregular singular point of the equation. It is not, therefore, possible to construct a convergent expansion for the wave function in this region; at best an asymptotic series can be obtained. For this purpose we must isolate the most rapidly oscillating part of the wave function as $x \to \infty$, i.e., the "controlling factor." The equation being linear and of second order, this factor may be expected to be an exponential. Thus we substitute

$$\psi(x) = e^{S(x)} \qquad (2)$$

and obtain for $S(x)$ the asymptotic equation

$$S'' + (S')^2 \sim cx^6 . \qquad (3)$$

Usually around an irregular singular point

$$S'' \ll (S')^2 , \qquad (4)$$

so that we get the approximate first-order equation valid around $x = \infty$:

$$(S')^2 \sim cx^6$$

giving

$$S(x) \sim \pm \tfrac{1}{4}\sqrt{c}\,x^4 , \qquad (5)$$

which ensures (4). For obvious reasons we choose the negative sign in (5). To ensure that (5) is the controlling factor of the exact solution we must check that the ansatz

$$S(x) = -\tfrac{1}{4}\sqrt{c}\,x^4 + d(x) , \qquad (6)$$

$$d(x) \ll \tfrac{1}{4}\sqrt{c}\,x^4 , \quad x \to \infty \qquad (7)$$

in the exact solution leads to an asymptotically valid relation for $d(x)$ which is less rapidly varying than (5). Substituting (6) in (2) and (1) leads to the equation

$$d'' - 3\sqrt{c}\,x^2 + (d')^2 - 2\sqrt{c}\,x^3 d' - bx^4 - ax^2 + E = 0 . \qquad (8)$$

However, (7) ensures that

$$d'' \ll 3\sqrt{c}\,x^2 , \quad (d')^2 \ll \sqrt{c}\,x^3 d'$$

so that asymptotically, we have

$$d' \sim \frac{-b}{2\sqrt{c}}\,x ,$$

i.e.,

$$d \sim \frac{-b}{4\sqrt{c}}\,x^2 , \quad x \to \infty . \qquad (9)$$

This establishes that (5) is, indeed, the controlling factor for the exact solution. Proceeding in this fashion, i.e., factoring out successively each leading oscillatory behavior, we obtain the complete leading behavior (i.e., the first term of the asymptotic series) of the wave function as

$$S(x) = -\frac{\sqrt{c}\,x^4}{4} - \frac{bx^2}{4\sqrt{c}} + \frac{(b^2 - 12c\sqrt{c} - 4ac)}{8c\sqrt{c}} \ln x . \qquad (10)$$

Introducing

$$\alpha = \sqrt{c} , \quad \beta = \frac{b}{2\sqrt{c}} , \quad \gamma = \frac{b^2 - 4ac}{4c\sqrt{c}} , \qquad (11)$$

we obtain

$$\psi(x) \sim x^{(\gamma-3)/2} \exp\left(-\frac{\alpha}{4}x^4 - \frac{\beta}{2}x^2\right) w(x) \text{ as } x \to \infty . \qquad (12)$$

To construct the full asymptotic series for $w(x)$ we write

$$w(x)=1+\epsilon(x)\,,\quad \epsilon(x)\to 0 \quad \text{as } x\to\infty\,, \tag{13}$$

i.e., we expect that $w(x)$ will be a power series in suitable inverse powers of x. Substitution of (12) in (1) leads to the asymptotic relation

$$\epsilon'\sim\frac{\delta}{2\sqrt{c}}x^{-3}\,, \tag{14}$$

where

$$\delta=E+\beta(2-\gamma) \tag{15}$$

so that

$$\epsilon\sim-\frac{\delta}{4\sqrt{c}}x^{-2}\,. \tag{16}$$

Equation (16) suggests that $w(x)$ is a power series in inverse powers of x^2; indeed, if we use the ansatz

$$w(x)=1-\frac{\delta}{4\sqrt{c}}x^{-2}+\epsilon_1(x) \tag{17}$$

we get the asymptotic relation

$$\epsilon_1(x)\sim\frac{1}{8\alpha}\left[\frac{(\gamma-3)(\gamma-5)}{4}-\frac{\delta^2}{4\alpha}-\frac{\delta\beta}{\alpha}\right]x^{-4}\,. \tag{18}$$

We therefore write

$$w(x)=\sum_{n=0}^{\infty}a_n x^{-2n}\,,\quad a_0=1\,,\quad a_{-1}=0\,. \tag{19}$$

Substitution in (12) and (1) leads to the difference equation

$$4\alpha(n+2)a_{n+2}+[E+4\beta(n+1)+\beta(2-\gamma)]a_{n+1}+[2n(2n+1)-2(\gamma-3)n+\tfrac{1}{4}(\gamma-3)(\gamma-5)]a_n=0 \tag{20}$$

The solution of (20) in the form of an infinite continued fraction is well known:

$$\frac{a_{K+1}}{a_K}=\cfrac{-[2K(2K+1)-2(\gamma-3)K+\frac{1}{4}(\gamma-3)(\gamma-5)]}{[E+4\beta(K+1)+\beta(2-\gamma)]-\cfrac{4\alpha(K+2)[(2K+2)(2K+3)-2(\gamma-3)(K+1)+\frac{1}{4}(\gamma-3)(\gamma-5)]}{[E+4\beta(K+2)+\beta(2-\gamma)]-\cdots}}\,. \tag{21}$$

That such equations constitute the eigenvalue condition has been observed[14]; for our purposes, the relation may be used to generate coefficients for the wave function provided the eigenvalue E has been determined by numerical methods. In practice, we expect a few terms in the series to give a good estimate of the wave function asymptotically.

From Eq. (21) we observe that for certain special values of γ, which is an expression involving the harmonic and anharmonic potential strengths, the infinite continued fraction terminates leading to a finite series expansion for $w(x)$. For, if γ satisfies the relation

$$2N(2N+1)-2(\gamma-3)N+\tfrac{1}{4}(\gamma-3)(\gamma-5)=0\,,$$

i.e.,

$$\gamma=4(N+1)\pm1\,,\quad N=0,1,2,\ldots \tag{22}$$

the coefficient a_{N+1} vanishes for $a_N\neq 0$. Equation (20) then ensures that subsequently all higher coefficients also vanish yielding the finite series

$$w(x)=\sum_{m=0}^{N}a_m x^{-2m}\,.$$

It is easily shown that for $\gamma=4N+3$, $N=0,1,2,3,\ldots$, the sequence of the finite series expansions given by

$$\psi(x)=x^{2N}\exp(-\tfrac{1}{4}\alpha x^4-\tfrac{1}{2}\beta x^2)\sum_{m=0}^{N}a_m x^{-2m}\,,$$

where the a_m's now satisfy the recurrence relation

$$4\alpha(m+2)a_{m+2}+[E+4\beta(m-N+1)-\beta]a_{m+1}+[2m(2m+1)-8Nm-2N(2N-1)]a_m=0\,, \tag{23}$$

provides exact polynomial solutions for the even-parity states of the doubly anharmonic system. The energy eigenvalue E is obtained as a root of an $(N+1)\times(N+1)$ determinant. A similar sequence of exact solutions for the odd-parity states of the system are obtained when γ takes the sequence of values $\gamma=4N+5$, $N=0,1,2,\ldots$.[24,25]

III. EXCITED ENERGY LEVELS: ASYMPTOTIC SERIES IN THE MAJOR COUPLING

We write the Hamiltonian for the system in the form

$$H(a,b,c)=-\frac{d^2}{dx^2}+ax^2+bx^4+cx^6\,. \tag{24}$$

Under the scaling transformation

$$x=c^{-1/8}y\,, \tag{25}$$

the Hamiltonian transforms as follows:

$$H(a,b,c)=c^{1/4}H(c^{-1/2}a,c^{-3/4}b,1)\,. \tag{26}$$

We are interested in the eigenvalues of this Hamiltonian as $c\to\infty$. In this limit

$$H(a,b,c)\sim c^{1/4}H(0,0,1)\,. \tag{27}$$

Since $H(0,0,1)$ is asymptotically independent of c, we may expect the energy levels of $H(a,b,c)$ to have the asymptotic form

$$E_n(a,b,c) \underset{c\to\infty}{\sim} A_n c^{1/4}, \tag{28}$$

where A_n may depend on n (the excitation quantum number) and on a and b. The Schrödinger equation for the energy eigenvalues transformed to the variable y as given by (25) is

$$\frac{d^2\psi}{dy^2} + (\mu - ac^{-1/2}y^2 - bc^{-3/4}y^4 - y^6)\psi = 0, \tag{29}$$

where

$$\mu = c^{-1/4}E(a,b,c). \tag{30}$$

The nth eigenvalue of this equation, in increasing order of magnitude, is denoted as μ_n.

Titchmarsh[23] has studied the nature and distribution of eigenvalues of the class of eigenvalue problems characterized by the equation

$$\frac{d^2\psi}{dx^2} + [\mu - q(x)]\psi = 0, \quad -\infty < x < \infty. \tag{31}$$

If $q(x) \to \infty$ as $x \to \pm\infty$, there is a purely point spectrum. For the distribution of eigenvalues, the approximation of the eigenfunctions by Bessel functions of order $\frac{1}{3}$ gives zero error formulas for the number of eigenvalues not exceeding a given number. In particular, for (31) with $q(x)$ having the given asymptotic behavior, he obtains the formula

$$n + \tfrac{1}{2} + O\left(\frac{1}{n}\right) = \frac{1}{\pi}\int_{x_n'}^{x_n} [\mu - q(x)]^{1/2} dx, \tag{32}$$

where x_n', x_n are roots of the equation

$$q(x) = \mu_n.$$

Applying (32) to (29), we have that for large n,

$$n + \tfrac{1}{2} \simeq \frac{\mu_n^{1/2}}{\pi}\int_{-y_0}^{y_0}\left(1 - \frac{ac^{-1/2}}{\mu_n}y^2 - \frac{bc^{-3/4}}{\mu_n}y^4 - \frac{y^6}{\mu_n}\right)^{1/2} dy. \tag{33}$$

Here y_0 is the real root closest to unity of the polynomial equation

$$\frac{y^6}{\mu_n} + \frac{bc^{-3/4}}{\mu_n}y^4 + \frac{ac^{-1/2}}{\mu_n}y^2 = 1. \tag{34}$$

We simplify (33) with the substitution $z = \mu_n^{-1/6}y$ to obtain

$$n + \tfrac{1}{2} \simeq \frac{\mu_n^{2/3}}{\pi}\int_{-z_0}^{z_0}(1 - z^6 - \rho z^4 - \sigma z^2)^{1/2} dz, \tag{35}$$

where

$$\rho = bc^{-3/4}\mu_n^{-1/3}, \quad \sigma = ac^{-1/2}\mu_n^{-2/3}. \tag{36}$$

z_0 is the root closest to unity of the transform of (34), i.e., of

$$z^6 + \rho z^4 + \sigma z^2 = 1. \tag{37}$$

Thus we may replace 1 by $z_0^6 + \rho z_0^4 + \sigma z_0^2$ in the integrand of (35) to obtain

$$n + \tfrac{1}{2} \simeq \frac{\mu_n^{2/3}}{\pi}\int_{-z_0}^{z_0}[(z_0^6 - z^6) + \rho(z_0^4 - z^4) + \sigma(z_0^2 - z^2)]^{1/2} dz. \tag{38}$$

Introducing the variable $u = z/z_0$, we have

$$n + \tfrac{1}{2} \simeq \frac{2}{\pi}\mu_n^{2/3}z_0^4\int_0^1[(1 - u^6) + \tau(1 - u^4) + \kappa(1 - u^2)]^{1/2} du, \tag{39}$$

where

$$\tau = \frac{\rho}{z_0^2}, \quad \kappa = \frac{\sigma}{z_0^4}. \tag{40}$$

We now examine the nature of (39), insofar as its dependence on μ_n, the energy eigenvalue, and the couplings a, b, c is concerned. Since ρ and σ depend on μ_n and the couplings a, b, c through (36), so does the root z_0 of Eq. (37). In (39) z_0 and the parameters τ and κ therefore have a well-defined dependence on μ_n and the couplings a, b, and c. We may therefore regard (39) as an implicit equation for μ_n in terms of the couplings, the relation being exact in the limit of large n. Our task is to solve this implicit relation to obtain μ_n as a power series in suitable inverse powers of c, the major coupling.

We first expand the root z_0 of (37) in inverse powers of c. Equation (37) can be rewritten as

$$z_0 = (1 - \rho z_0^4 - \sigma z_0^2)^{1/6}. \tag{41}$$

From (28) and (30) we find that $\mu_n \to$ a constant as $c \to \infty$; thus from (36) $\rho, \sigma \to 0$ in the same limit. We may therefore expand the right-hand side of (41) in powers of ρ and σ and write

$$\begin{aligned} z_0 = [1 &- \tfrac{1}{6}\rho(1 - \rho z_0^4 - \sigma z_0^2)^{2/3} - \tfrac{1}{6}\sigma(1 - \rho z_0^4 - \sigma z_0^2)^{1/3} \\ &- \tfrac{5}{72}\sigma^2(1 - \rho z_0^4 - \sigma z_0^2)^{2/3} - \tfrac{5}{36}\rho\sigma(1 - \rho z_0^4 - \sigma z_0^2) \\ &- \tfrac{5}{72}\rho^2(1 - \rho z_0^4 - \sigma z_0^2)^{4/3} + \cdots]. \end{aligned} \tag{42}$$

Substituting once more for z_0 from (41) in the right-hand side of (42) we obtain z_0 as an expansion in inverse powers of $c^{1/4}$:

$$\begin{aligned} z_0 &= 1 - \frac{\sigma}{6} - \frac{\rho}{6} - \frac{\sigma^2}{72} - \frac{\sigma\rho}{36} + \frac{\rho^2}{24} + \cdots \\ &= 1 - \frac{a\mu_n^{-2/3}}{6}c^{-1/2} - \frac{b\mu_n^{-1/3}}{6}c^{-3/4} - \cdots. \end{aligned} \tag{43}$$

Since $z_0 \to 1$ for large c, we expand (39) as a power series in τ and κ which, by virtue of (36) and (40), is a series in inverse powers of $c^{1/4}$. We first obtain

$$n + \frac{1}{2} \simeq \frac{2}{\pi}\mu_n^{2/3}z_0^4\left(J_1 + \frac{\tau}{2}J_2 + \frac{\kappa}{2}J_3 - \frac{\kappa^2}{8}J_4 + \cdots\right). \tag{44}$$

Here the J_i's are definite integrals related to the elliptic integrals

$$J_1 \equiv \int_0^1 (1-u^6)^{1/2}du ,$$

$$J_2 \equiv \int_0^1 (1-u^6)^{-1/2}(1-u^4)du ,$$

$$J_3 \equiv \int_0^1 (1-u^6)^{-1/2}(1-u^2)du ,$$

$$J_4 \equiv \int_0^1 (1-u^6)^{-3/2}(1-u^2)^2du ,$$

and we have retained terms which contribute to the energy eigenvalue to $O(c^{-1})$. Each of these integrals is finite and may be evaluated by elementary means using the integral representation for the beta function

$$B(\mu,\nu)=\int_0^1 (1-x)^{\mu-1}x^{\nu-1}dx\,, \quad \mathrm{Re}\mu>0, \quad \mathrm{Re}\nu>0$$

and its analytic continuation to $\mathrm{Re}\mu<0$. We obtain

$$\begin{aligned} J_1&=\frac{\sqrt{\pi}}{8}\,\frac{\Gamma(\frac{1}{6})}{\Gamma(\frac{2}{3})}\,, \quad J_2=\frac{\sqrt{\pi}\,\Gamma(\frac{1}{6})-3\times 2^{1/3}\Gamma^2(\frac{5}{6})}{6\Gamma(\frac{2}{3})}\,,\\ J_3&=\frac{1}{6}\left[\frac{\sqrt{\pi}\,\Gamma(\frac{1}{6})}{\Gamma(\frac{2}{3})}-\pi\right],\\ J_4&=\frac{1}{18\Gamma(\frac{2}{3})}\,[2\sqrt{\pi}\,\Gamma(\tfrac{1}{6})-3\times 2^{2/3}\Gamma^2(\tfrac{5}{6})]\,. \end{aligned} \tag{45}$$

Inverting (39) and expanding the result in powers of τ and κ, we have

$$\mu_n\simeq (n+\tfrac{1}{2})^{3/2}\left(\frac{\pi}{2}\right)^{3/2} \times z_0^{-6}J_1^{-3/2}\left(1-\frac{3}{4}\tau\frac{J_2}{J_1}-\frac{3}{4}\kappa\frac{J_3}{J_1}+\frac{3}{16}\kappa^2\frac{J_4}{J_1}+\cdots\right). \tag{46}$$

Using (43) and (40) we have

$$\begin{aligned} z_0^{-6}\tau&=\rho(1+\tfrac{4}{3}\sigma+\tfrac{4}{3}\rho+\cdots)\,,\\ z_0^{-6}\kappa&=\sigma(1+\tfrac{5}{3}\sigma+\tfrac{5}{3}\rho+\cdots)\,,\\ z_0^{-6}\kappa^2&=\sigma^2(1+\tfrac{7}{3}\sigma+\cdots)\,, \end{aligned} \tag{47}$$

which on substitution in (46) leads to the result

$$\mu_n\simeq (n+\tfrac{1}{2})^{3/2}\left(\frac{\pi}{2}\right)^{3/2} \times J_1^{-3/2}\left[1+\sigma\left(1-\frac{3}{4}\frac{J_3}{J_1}\right)+\rho\left(1-\frac{3}{4}\frac{J_2}{J_1}\right) +\sigma^2\left(\frac{2}{3}-\frac{5}{4}\frac{J_3}{J_1}+\frac{3}{16}\frac{J_4}{J_1}+\frac{15}{32}\frac{J_3^{\,2}}{J_1^{\,2}}\right)+\cdots\right]. \tag{48}$$

Using (36) we get the implicit equation giving μ_n in terms of known integrals and inverse powers of $c^{1/4}$:

$$\mu_n\simeq (n+\tfrac{1}{2})^{3/2}\left(\frac{\pi}{2}\right)^{3/2}J_1^{-3/2}\left[1+\frac{ac^{-1/2}}{\mu_n^{2/3}}\left(1-\frac{3}{4}\frac{J_3}{J_1}\right)+\frac{bc^{-3/4}}{\mu_n^{1/3}}\left(1-\frac{3}{4}\frac{J_2}{J_1}\right) +\frac{a^2c^{-1}}{\mu_n^{4/3}}\left(\frac{2}{3}-\frac{5}{4}\frac{J_3}{J_1}+\frac{3}{16}\frac{J_4}{J_1}+\frac{15}{32}\frac{J_3^2}{J_1^{\,2}}\right)+\cdots\right]. \tag{49}$$

μ_n as a powers series in $c^{-1/4}$ is obtained by successive iteration of this equation. Thus if $\mu_n^{(i)}$ is the asymptotic expression for μ_n at the $(i+1)$th iteration,

$$\mu_n^{(i)}=(n+\tfrac{1}{2})^{3/2}\left(\frac{\pi}{2}\right)^{3/2}J_1^{-3/2}\left[1+\frac{ac^{-1/2}}{[\mu_n^{(i-1)}]^{2/3}}\left(1-\frac{3}{4}\frac{J_3}{J_1}\right)+\cdots\right],$$

the series being terminated at the $(i+1)$th term, with $\mu_n^{(0)}=(n+\frac{1}{2})^{3/2}(\frac{1}{2}\pi)^{3/2}J_1^{-3/2}$. The structure of the implicit equation (49) ensures that the coefficient of a given power of $c^{-1/4}$ is uniquely determined by a finite number of iterations, subsequent iterations leaving coefficients of lower powers undisturbed. We thus obtain the asymptotic series for μ_n which, in conjunction with (30), yields

$$E_n(a,b,c)\simeq c^{1/4}(A_n+B_nc^{-1/2}+C_nc^{-3/4} +D_nc^{-1}+\cdots)\,, \tag{50}$$

where

$$A_n=4(n+\tfrac{1}{2})^{3/2}\frac{\Gamma^3(\frac{2}{3})}{\Gamma^{3/2}(\frac{1}{3})}\,,$$

$$\begin{aligned} B_n&=a(n+\tfrac{1}{2})^{1/2}\frac{\Gamma^3(\frac{2}{3})}{\Gamma^{3/2}(\frac{1}{3})}\,,\\ C_n&=6b(n+\tfrac{1}{2})\frac{\Gamma^5(\frac{2}{3})}{\Gamma^4(\frac{1}{3})}\,,\\ D_n&=\frac{a^2}{4}(n+\tfrac{1}{2})^{-1/2}\left[\frac{1}{6}\frac{\Gamma^3(\frac{2}{3})}{\Gamma^{3/2}(\frac{1}{3})}-\frac{\Gamma^2(\frac{2}{3})}{\Gamma^{5/2}(\frac{1}{3})}\right]. \end{aligned} \tag{51}$$

We expect that in the large (c,n) domain a few terms in the series will give accurate values for E_n. For sufficiently large c the eigenvalues are determined by c alone, since A_n is independent of the couplings a and b; also the series (50) reduces to that for the λx^6 oscillator for $b=0$. We note that in obtaining the series, the only assumption that has been made about the analytic structure of

$E_n(a,b,c)$ as $c \to \infty$ is that $\mu_n \to$ a constant as $c \to \infty$ (which follows from the scaling argument). The series results from the expansion of a convergent integral in terms of certain parameters on which it depends. Thus, while the analytic structure of the energy eigenvalues of the system in the major coupling is not known, the validity of the series does not depend on this knowledge. However, a proof that this series is truly asymptotic depends on our understanding of the dependence on the couplings of the corrections to the Titchmarsh expression. In the absence of such a proof, numerical calculations have been used to test the accuracy of the series.

IV. NUMERICAL ANALYSIS: ACCURACY OF THE ASYMPTOTIC SERIES

The accuracy of the asymptotic series (50) for the energy eigenvalues remains to be established. Since no analytic solution of the energy-eigenvalue problem exists, we examine the question numerically. However, numerical solutions for the energy eigenvalues corresponding to the excited states of doubly anharmonic oscillators are not available in the literature; we are, therefore, forced to compute (numerically) the exact eigenvalues and compare them with the result of the asymptotic series (50).

To compute the exact energy eigenvalues we employ the method based on the use of the truncated Hill determinant,[4] modified by the use of scaled basis functions.[5] The truncated Hill determinant has been used earlier with considerable success in studying the energy levels of anharmonic oscillators of the λx^{2m} type.[4] Using for the wave function of the nth energy level the ansatz

$$\psi_n(x) = e^{-\bar{\lambda}(n,c)x^2} \sum_{m=0}^{\infty} a_m x^{2m+v}, \qquad (52)$$

where $\bar{\lambda}(n,c)$ is a scaling parameter to be (subsequently) chosen and $v=0$ ($v=1$) for states of even (odd) parity, we obtain for the a_m's a 5-contiguous-term difference equation. The consistency condition for the existence of a nontrivial set of a_m's is the vanishing of the Hill determinant. We truncate this determinant at a finite order; the resulting consistency equation is a polynomial in E, the energy eigenvalue, with coefficients which are functions of the couplings a, b, and c. Choosing suitable values of these couplings we look for the roots of this polynomial numerically. The recursion relation between successive truncations of the Hill determinant enables us to locate the root of successively higher-order polynomials: the stability of the root as one passes to polynomials of higher order is taken to establish the location of the true eigenvalues as roots of the Hill determinant.

The choice of the scaling parameter $\bar{\lambda}(n,c)$ is determined as follows. We wish to choose $\bar{\lambda}$ in a way such that the first n members of the basis functions, viz., $a_m e^{-\bar{\lambda}x^2} x^{2m}$ $(m=0,1,\ldots,n)$, have

TABLE I. Eigenvalues of the $ax^2+bx^4+cx^6$ oscillator compared with the result of the four-term asymptotic series. In these tables n is the excitation number of the level, λ_E is the exact eigenvalue, λ_A is the result obtained from the four-term asymptotic series, and δ_E is the relative error defined as $\delta_E \equiv (\lambda_E - \lambda_A)/\lambda_E$. We take $a=b=c=1$.

n	λ_E	λ_A	δ_E
1	5.656	5.637	0.336×10^{-2}
2	11.107	11.165	-0.522×10^{-2}
3	17.637	17.739	-0.578×10^{-2}
4	25.068	25.203	-0.538×10^{-2}
5	33.293	33.455	-0.486×10^{-2}
6	42.236	42.421	-0.438×10^{-2}
7	51.841	52.047	-0.397×10^{-2}
8	62.062	62.286	-0.361×10^{-2}
9	72.861	73.103	-0.332×10^{-2}
10	84.209	84.466	-0.305×10^{-2}
20	223.295	223.673	-0.169×10^{-2}
30	400.371	400.836	-0.116×10^{-2}
40	608.349	608.886	-0.882×10^{-3}
50	843.079	843.678	-0.710×10^{-3}
60	1101.739	1102.395	-0.595×10^{-3}
70	1382.253	1382.959	-0.510×10^{-3}
80	1683.005	1683.758	-0.447×10^{-3}
90	2002.692	2003.490	-0.398×10^{-3}
100	2340.237	2341.076	-0.358×10^{-3}

TABLE II. Same as Table I but with $a=b=1$, $c=5$.

n	λ_E	λ_A	δ_E
1	7.279	7.038	0.331×10^{-1}
2	14.731	14.577	0.104×10^{-1}
3	23.837	23.714	0.513×10^{-2}
4	34.303	34.201	0.295×10^{-2}
5	45.965	45.879	0.186×10^{-2}
6	58.709	58.636	0.124×10^{-2}
7	72.447	72.384	0.870×10^{-3}
8	87.111	87.056	0.628×10^{-3}
9	102.644	102.596	0.462×10^{-3}
10	118.999	118.958	0.346×10^{-3}
20	320.960	320.958	0.478×10^{-5}
30	579.833	579.853	-0.357×10^{-4}
40	884.971	885.007	-0.415×10^{-4}
50	1230.147	1230.196	-0.401×10^{-4}
60	1611.134	1611.194	-0.373×10^{-4}
70	2024.818	2024.888	-0.343×10^{-4}
80	2468.780	2468.858	-0.315×10^{-4}
90	2941.071	2941.156	-0.290×10^{-4}
100	3440.074	3440.167	-0.268×10^{-4}

TABLE III. Same as Table I but with $a=b=1$, $c=10$.

n	λ_E	λ_A	δ_E
1	8.346	8.039	0.368×10^{-1}
2	17.046	16.843	0.119×10^{-1}
3	27.726	27.556	0.614×10^{-2}
4	40.027	39.879	0.368×10^{-2}
5	53.754	53.623	0.243×10^{-2}
6	68.769	68.651	0.171×10^{-2}
7	84.969	84.861	0.126×10^{-2}
8	102.271	102.172	0.965×10^{-3}
9	120.608	120.516	0.759×10^{-3}
10	139.924	139.839	0.609×10^{-3}
20	378.794	378.745	0.129×10^{-3}
30	685.381	685.350	0.446×10^{-4}
40	1047.005	1046.987	0.176×10^{-4}
50	1456.256	1456.246	0.649×10^{-5}
60	1908.102	1908.100	0.116×10^{-5}
70	2398.838	2398.842	-0.160×10^{-5}
80	2925.586	2925.595	-0.310×10^{-5}
90	3486.027	3486.041	-0.392×10^{-5}
100	4078.239	4078.257	-0.437×10^{-5}

TABLE V. Same as Table I but with $a=b=1$, $c=50$.

n	λ_E	λ_A	δ_E
1	11.913	11.438	0.399×10^{-1}
2	24.651	24.332	0.129×10^{-1}
3	40.374	40.100	0.679×10^{-2}
4	58.528	58.286	0.413×10^{-2}
5	78.821	78.603	0.277×10^{-2}
6	101.046	100.845	0.198×10^{-2}
7	125.046	124.859	0.149×10^{-2}
8	150.697	150.522	0.116×10^{-2}
9	177.899	177.734	0.928×10^{-3}
10	206.567	206.410	0.759×10^{-3}
20	561.672	561.562	0.196×10^{-3}
30	1018.112	1018.023	0.875×10^{-4}
40	1556.893	1556.817	0.489×10^{-4}
50	2166.916	2166.849	0.310×10^{-4}
60	2840.653	2840.592	0.213×10^{-4}
70	3572.558	3572.502	0.154×10^{-4}
80	4358.324	4358.273	0.116×10^{-4}
90	5194.481	5194.434	0.911×10^{-5}
100	6078.155	6078.111	0.727×10^{-5}

appreciable values in the region of oscillation of the actual nth eigenfunction. The WKB estimate of this region of oscillation is $n^{1/4}c^{-1/8}$. This is therefore set equal to the width of the nth basis function, i.e., $n^{1/2}\bar{\lambda}^{-1/2}$. Thus one obtains

$$\bar{\lambda}(n,c)\sim n^{1/2}c^{1/4}.$$

For the pure harmonic case, $\bar{\lambda}=\frac{1}{2}$. We therefore use the following scaling formula for $\bar{\lambda}$:

$$\bar{\lambda}(n,c)=\tfrac{1}{2}+An^{1/2}c^{1/4}. \tag{53}$$

A is a constant empirically chosen as 1.5. Equation (52) used in conjunction with (53) in (1) yields the difference equation

$$a_{m+1}+p_m a_m+q_m a_{m-1}+r_m a_{m-2}+s_m a_{m-3}=0\,, \tag{54}$$

with

TABLE IV. Same as Table I but with $a=b=1$, $c=20$.

n	λ_E	λ_A	δ_E
1	9.679	9.304	0.387×10^{-1}
2	19.904	19.653	0.126×10^{-1}
3	32.493	32.280	0.657×10^{-2}
4	47.014	46.826	0.398×10^{-2}
5	63.233	63.065	0.266×10^{-2}
6	80.987	80.833	0.189×10^{-2}
7	100.150	100.008	0.142×10^{-2}
8	120.626	120.493	0.109×10^{-2}
9	142.334	142.209	0.874×10^{-3}
10	165.207	165.089	0.712×10^{-3}
20	448.326	448.247	0.176×10^{-3}
30	812.006	811.945	0.745×10^{-4}
40	1241.153	1241.104	0.395×10^{-4}
50	1726.948	1726.907	0.236×10^{-4}
60	2263.406	2263.371	0.153×10^{-4}
70	2846.118	2846.088	0.104×10^{-4}
80	3471.660	3471.635	0.728×10^{-5}
90	4137.273	4137.252	0.528×10^{-5}
100	4840.673	4840.654	0.381×10^{-5}

TABLE VI. Same as Table I but with $a=b=1$, $c=100$.

c	λ_E	λ_A	δ_E
1	14.023	13.457	0.403×10^{-1}
2	29.109	28.729	0.130×10^{-1}
3	47.749	47.421	0.686×10^{-2}
4	69.283	68.994	0.418×10^{-2}
5	93.364	93.102	0.280×10^{-2}
6	119.743	119.502	0.201×10^{-2}
7	148.234	148.010	0.151×10^{-2}
8	178.689	178.479	0.117×10^{-2}
9	210.989	210.790	0.942×10^{-3}
10	245.033	244.844	0.771×10^{-3}
20	666.871	666.736	0.201×10^{-3}
30	1209.237	1209.128	0.906×10^{-4}
40	1849.536	1849.441	0.511×10^{-4}
50	2574.563	2574.479	0.327×10^{-4}
60	3375.364	3375.288	0.227×10^{-4}
70	4245.344	4245.273	0.166×10^{-4}
80	5179.378	5179.313	0.126×10^{-4}
90	6173.341	6173.280	0.999×10^{-5}
100	7223.813	7223.755	0.806×10^{-5}

TABLE VII. Same as Table I but with $a=1$, $b=-1$, $c=10$ ($b^2<3ac$).

n	λ_E	λ_A	δ_E
2	16.221	16.004	0.13×10^{-1}
4	38.533	38.370	0.42×10^{-2}
6	66.604	66.471	0.20×10^{-2}
8	99.435	99.321	0.11×10^{-2}
10	136.417	136.317	0.73×10^{-3}

TABLE IX. Same as Table I but with $a=0.1$, $b=-2$, $c=10$ ($b^2=4ac$).

n	λ_E	λ_A	δ_E
2	15.315	15.133	0.12×10^{-1}
4	37.134	37.009	0.34×10^{-2}
6	64.742	64.651	0.14×10^{-2}
8	97.128	97.061	0.69×10^{-3}
10	133.677	133.628	0.37×10^{-3}

$$p_m=\frac{E-2\bar{\lambda}(4m+2v+1)}{(2m+2+v)(2m+1+v)}\,,\quad q_m=\frac{4\bar{\lambda}^2-a}{(2m+2+v)(2m+1+v)}\,,\quad r_m=\frac{-b}{(2m+2+v)(2m+1+v)}\,,\quad s_m=\frac{-c}{(2m+2+v)(2m+1+v)}\,. \tag{55}$$

The eigenvalues are now roots of the Hill determinant

$$\Delta(E)\equiv\begin{vmatrix} p_0 & 1 & 0 & 0 & 0 & 0 & 0 & \cdots \\ q_1 & p_1 & 1 & 0 & 0 & 0 & 0 & \\ r_2 & q_2 & p_2 & 1 & 0 & 0 & 0 & \\ s_3 & r_3 & q_3 & p_3 & 1 & 0 & 0 & \\ 0 & s_4 & r_4 & q_4 & p_4 & 1 & 0 & \\ \cdot & & & & & & & \cdot \\ \cdot & & & & & & & \cdot \\ \cdot & & & & & & & \cdot \end{vmatrix}\,. \tag{56}$$

If Δ_m stands for the $m\times m$ approximant to (56), the Δ_m's satisfy the recursion relation

$$\Delta_{m+1}-p_m\Delta_m+q_m\Delta_{m-1}-r_m\Delta_{m-2}+s_m\Delta_{m-3}=0\quad(\Delta_0=1)\,. \tag{57}$$

We use (57) to generate higher-order approximants to the Hill determinant. The limit (if any) of the sequence of roots of Δ_m as $m\to\infty$ is the required eigenvalue. In actual practice, the zeros of $\Delta_m(E)$, which is an mth-order polynomial in E, stabilize for large m. For $n=100$ and $c=100$ ($a=1$, $b=1$) it is possible to obtain a root stable to one part in 10^9 with $m=250$.

The results of the calculations are given in Tables I–X. The asymptotic series is truncated at the 4th term, i.e., as given in (50). For $b>0$, the accuracy of the four-term series increases, in general, with the magnitude of the major coupling (c) and with the excitation number of the level being compared. An accuracy of 1 part in one million is achieved for $c=10$, $a=b=1$ at the 60th excited state.

We have also examined the accuracy of the series for $b<0$. Where for $b>0$ the potential function $V(x)=ax^2+bx^4+cx^6$ ($a,c>0$) has no extrema, for $b<0$ the potential function has maxima and minima depending on the relative magnitudes of b^2 and ac. Thus, for $b^2<3ac$ no extrema appear; a point of inflection appears at $b^2=3ac$; for $3ac<b^2<4ac$ two positive minima (and maxima) located symmetrically about $x=0$ are to be seen. Finally, the minima are tangent to the $V(x)=0$ for $b^2=4ac$ and are negative for $b^2>4ac$. We find (Tables VII–IX) the accuracy of the series in these cases to be comparable to those for $b>0$; however, for large and negative b ($b<0:b^2>4ac$) the constraint $|b|/c\ll1$ is violated and we do not expect the series to be accurate for the low-lying levels. We have consequently not used the asymptotic series to estimate the eigenvalues when b is negative and large in magnitude.

For $b=0$ the asymptotic series expansion reduces to that for a λx^6 oscillator and the accuracy remains comparable to that in the situations when

TABLE VIII. Same as Table I but with $a=0.3$, $b=-3$, $c=10$ ($b^2=3ac$).

n	λ_E	λ_A	δ_E
2	14.962	14.815	0.98×10^{-2}
4	36.470	36.389	0.22×10^{-2}
6	63.760	63.723	0.57×10^{-3}
8	95.825	95.820	0.52×10^{-4}
10	132.053	132.073	-0.15×10^{-3}

TABLE X. Same as Table I but with $a=1$, $b=0$, $c=1$.

n	λ_E	λ_A	δ_E
2	9.966	9.839	0.13×10^{-1}
4	22.910	22.816	0.41×10^{-2}
6	39.059	38.974	0.20×10^{-2}
8	57.845	57.778	0.12×10^{-2}
10	78.958	78.897	0.76×10^{-3}

$b \neq 0$, as is to be seen in Table X.

We therefore conclude that the asymptotic series (50), truncated after a few (~5) terms, gives the energy levels of the doubly anharmonic oscillator with considerable accuracy for all states except the ground state. Indeed, for any "exact" numerical evaluation, the asymptotic series provides an excellent starting point.

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