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Quantum solution for the biharmonic oscillator

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The quantum-mechanical solution for the biharmonic oscillator is presented. This one-dimensional asymmetric oscillator is described by the potential energy function $V(x) = m\omega_1{}^2/2$, $x > 0$, and $V(x) = m\omega_2{}^2/2$, $x < 0$. One of the more interesting features of the solution is that the energy levels are very nearly equally spaced. The biharmonic oscillator provides a relatively simple model for systems which lack the symmetry of the harmonic oscillator.

Of the models used in both classical and quantum mechanics, the harmonic oscillator is probably more widely employed than any other. The symmetry of the potential energy function about its minimum is one of the simplifying features of the harmonic oscillator. Yet this symmetry is one which is seldom present in the physical system for which the oscillator is the model. For example, many real springs have different force constants for extension and for compression from the equilibrium length, and more realistic models of interatomic potentials in solids, liquids, and gases use potential energy forms which are not symmetric about the position of the minimum. A relatively simple model which lacks this symmetry would be valuable.

We consider here the quantum-mechanical solution of the *biharmonic* oscillator—a harmonic oscillator in each half-space. The oscillator frequency is ω_1 for $x > 0$ and ω_2 for $x < 0$. With a mass m and the usual step function $S(x)$, we have the potential energy function,

$$V = \tfrac{1}{2} m x^2 [\omega_1{}^2 S(x) + \omega_2{}^2 S(-x)]. \tag{1}$$

We have not found any mention of this problem in the recent literature. Even if it has received attention in the past, we think it worth reviving for a number of reasons, including the following: The biharmonic oscillator has pedagogic interest as a solvable quantum-mechanical problem. Containing the harmonic oscillator as a special case, it provides some insight into the solution of that simpler case. From a practical standpoint, the biharmonic oscillator may be used successfully as a better model for many of those systems usually treated in a harmonic approximation. For example, the classical statistical thermodynamics of a linear chain of masses interacting via these biharmonic springs has been considered.[1] Such an asymmetric interatomic potential leads quite naturally to thermal expansion without the necessity for introducing troublesome anharmonic corrections.

The quantum solution for the biharmonic oscillator is obtained by solving the Schrödinger equation in each half-space and matching the solutions at $x = 0$. In an obvious notation, we have

$$\begin{aligned} \frac{d^2\psi_1}{dx^2} + \left(\frac{2mE}{\hbar^2} - \frac{m^2\omega_1{}^2 x^2}{\hbar^2}\right)\psi_1 &= 0, \quad x > 0, \\ \frac{d^2\psi_2}{dx^2} + \left(\frac{2mE}{\hbar^2} - \frac{m^2\omega_2{}^2 x^2}{\hbar^2}\right)\psi_2 &= 0, \quad x < 0, \end{aligned} \tag{2}$$

In each half-space, the customary change of variable and substitution are made. So, for $x > 0$, we let

$$\xi = (m\omega_1/\hbar)^{1/2} x, \quad \psi_1(x) = \exp(-\tfrac{1}{2}\xi^2) f(\xi)$$

and

$$\frac{d^2 f}{d\xi^2} - 2\xi \frac{df}{d\xi} + 2\mu f = 0, \quad E = (\mu + \tfrac{1}{2})\hbar\omega_1. \tag{3}$$

Similar expressions are obtained for $x < 0$. In particular, the parameter ν is the counterpart of μ in expressing the energy eigenvalue in terms of ω_2 rather than ω_1. Thus,

$$(\nu + \tfrac{1}{2})\hbar\omega_2 = (\mu + \tfrac{1}{2})\hbar\omega_1, \tag{4}$$

and the dependence of μ and ν is determined by the ratio of frequencies.

Continuing with the solution of the differential equation for $x > 0$, we have from Eq. (3) and the variable change $z = \xi^2$, $F(z) = f(\xi)$

$$z \frac{d^2 F}{dz^2} + (\tfrac{1}{2} - z)\frac{dF}{dz} + \frac{\mu}{2} F = 0,$$

which is the confluent hypergeometric equation with independent solutions[2]

$${}_1F_1(-\mu/2, \tfrac{1}{2}; z), \quad z^{1/2}\,{}_1F_1(\tfrac{1}{2} - \mu/2, \tfrac{3}{2}; z). \tag{5}$$

An arbitrary linear combination of these functions becomes unbounded as e^z for large z. It is at this point for the *harmonic* oscillator that the symmetry about $x = 0$ is invoked since the first of the solutions in Eq. (5) contains only even powers of x ($z = m\omega_1 x^2/\hbar$) and the second only odd powers of x. Thus μ is chosen to be an even or odd integer, leading respectively to even or odd polynomials in x.

For the *biharmonic* oscillator, this symmetry is absent and the linear combination of the functions of Eq. (5)

must be chosen so that a bounded solution is obtained for the wave function in the half-space $x > 0$. This linear combination is[2]

$$\Psi\left(-\frac{\mu}{2}, \frac{1}{2}, \frac{m\omega_1 x^2}{\hbar}\right) = \frac{\Gamma(\frac{1}{2})\,{}_1F_1(-\mu/2, \frac{1}{2}; m\omega_1 x^2/\hbar)}{\Gamma(\frac{1}{2}-\mu/2)} + \frac{\Gamma(-\frac{1}{2})(m\omega_1/\hbar)^{1/2} x\,{}_1F_1(\frac{1}{2}-\mu/2, \frac{3}{2}; m\omega_1 x^2/\hbar)}{\Gamma(-\mu/2)}$$

which behaves for large x as x^{μ}. The appropriate combination for the half-space $x < 0$ is

$$\Psi\left(-\frac{\nu}{2}, \frac{1}{2}, \frac{m\omega_2 x^2}{\hbar}\right) = \frac{\Gamma(\frac{1}{2})\,{}_1F_1(-\nu/2, \frac{1}{2}; m\omega_2 x^2/\hbar)}{\Gamma(\frac{1}{2}-\nu/2)} - \frac{\Gamma(-\frac{1}{2})(m\omega_2/\hbar)^{1/2} x\,{}_1F_1(\frac{1}{2}-\nu/2, \frac{3}{2}; m\omega_2 x^2/\hbar)}{\Gamma(-\nu/2)}.$$

Attaching the exponential factors and a multiplicative constant, we have then the solution of the Schroedinger equation in each half-space,

$$\psi_1 = A\Psi(-\mu/2, \tfrac{1}{2}, m\omega_1 x^2/\hbar) \times \exp(-\tfrac{1}{2} m\omega_1 x^2/\hbar), \qquad x > 0$$
$$\psi_2 = B\Psi(-\nu/2, \tfrac{1}{2}, m\omega_2 x^2/\hbar) \times \exp(-\tfrac{1}{2} m\omega_2 x^2/\hbar), \qquad x < 0. \tag{6}$$

These solutions are simply related to the parabolic cylinder functions.[2,3]

The energy eigenvalues are determined from a match in value and slope of the solutions at $x = 0$, leading to

$$\frac{\Gamma(\frac{1}{2}-\mu/2)}{\Gamma(-\mu/2)} = -\frac{(\omega_2/\omega_1)^{1/2}\Gamma(\frac{1}{2}-\nu/2)}{\Gamma(-\nu/2)},$$
$$(\nu+\tfrac{1}{2})\hbar\omega_2 = E = (\mu+\tfrac{1}{2})\hbar\omega_1.$$

A more convenient form is obtained by using two gamma function relations,[2]

$$\Gamma(z)\Gamma(1-z) = \pi\csc(\pi z),$$
$$\Gamma(\tfrac{1}{2}+z)\Gamma(\tfrac{1}{2}-z) = \pi\sec(\pi z).$$

The eigenvalues are determined then from the roots of

$$\tan\left(\frac{\pi\mu}{2}\right)\frac{\Gamma(1+\mu/2)}{\Gamma(\frac{1}{2}+\mu/2)} + \left(\frac{\omega_2}{\omega_1}\right)^{1/2}\tan\left(\frac{\pi\nu}{2}\right)\frac{\Gamma(1+\nu/2)}{\Gamma(\frac{1}{2}+\nu/2)} = 0, \tag{7}$$

with $\nu = (\mu + ½)\omega_1/\omega_2 - ½$.

Equation (7) admits the special solutions for the *harmonic* oscillator with $\omega_1 = \omega_2$, $\mu = \nu = n$, a nonnegative integer. Another special case is the half-oscillator, obtained in the limit $\omega_2/\omega_1 \to \infty$. Then, $\mu = 1, 3, 5$, etc.

For the general *biharmonic* oscillator, we note that the arguments of the gamma functions in Eq. (7) are nonnegative since $E = (\mu + ½)\hbar\omega_1 = (\nu + ½)\hbar\omega_2$ must be positive. Furthermore, the two tangent functions must have opposite signs to yield a root. The roots must be obtained by a numerical search, and for this purpose it is convenient to take $\omega_2 > \omega_1$. Thus, $\mu > \nu = (\mu + ½)\omega_1/\omega_2 - ½$. The tangent functions require that the integer portions of μ and ν differ by an odd integer, $[\mu] - [\nu] = 1, 3, 5, \ldots$. A consistent search procedure can then be developed by assigning to μ trial values between k and $k + 1$, $k = 0, 1, 2, \ldots$, calculating the trial value of $\nu = (\mu + ½)\omega_1/\omega_2 - ½$ and ascertaining that $[\mu] - [\nu]$ is an odd integer with the further restriction that $\nu > -½$ for a positive energy eigenvalue. For example, with $\omega_2 = 2\omega_1$ and $k = 0$, the maximum values of μ and ν, respectively, are 0.5 and 0^- while the minimum values in this range are 0^+ and -0.25, respectively. So μ must lie between 0 and 0.5. The actual value for this ground state root is $\mu_0 = 0.1786$ ($\nu_0 = -0.1607$). In a similar way the first excited state root value for μ must lie between 1 and 2 with ν between 0.25 and 0.75. The root values are $\mu_1 = 1.4934$, $\nu_1 = 0.4967$. As another example of the search procedure, if we consider a trial value of μ between 3 and 4, the trial values of ν would lie between 1.25 and 1.75 and $[\mu] - [\nu] = 2$, not an odd integer. Thus, no root exists for μ between 3 and 4.

The determination of the eigenvalues requires the evaluation of gamma function values. These can be obtained by using the property $\Gamma(z + 1) = z\Gamma(z)$ repeatedly and the asymptotic expansion[2]

$$\ln\Gamma(z) = (z - \tfrac{1}{2})\ln(z) - z + \tfrac{1}{2}\ln(2\pi) + z^{-1}/12 - z^{-3}/360 + z^{-5}/1260 + \cdots, \tag{8}$$

which is accurate to 1 part in 10^6 for z as small as 4.

By way of illustration, we display in Table I information on the first few eigenvalues for the biharmonic oscillator with $\omega_2 = 1.5\omega_1$. Listed are a counting index n

Table I. Energy level parameters for $\omega_2 = 1.5\omega_1$

n	μ_n	ν_n	$\mu_n + \nu_n - 2n$
0	0.1038	−0.0975	0.0063
1	1.2974	0.6983	−0.0043
2	2.5014	1.5009	0.0023
3	3.6994	2.2996	−0.0010
4	4.9002	3.1001	0.0003
5	6.1001	3.9001	0.0002
6	7.2998	4.6999	−0.0003
7	8.5002	5.5001	0.0003
8	9.6999	6.2999	−0.0002
9	10.9000	7.1000	0.0000

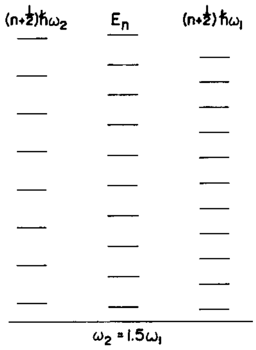

Fig. 1. The energy levels of the biharmonic oscillator with $\omega_2 = 1.5\omega_1$ are shown in the center column. The levels on the left are for a harmonic oscillator of frequency ω_2, while those on the right are for a harmonic oscillator of frequency ω_1. The biharmonic oscillator levels are almost equally spaced.

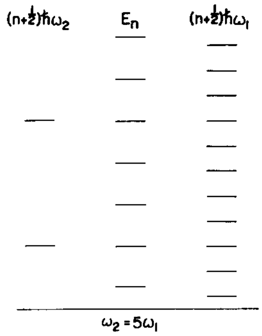

Fig. 2. The energy levels of the biharmonic oscillator with $\omega_2 = 5\omega_1$ are shown in the center column. The levels on the left are for a harmonic oscillator of frequency ω_2, while those on the right are for a harmonic oscillator of frequency ω_1. Since $\omega_2/\omega_1 = 5/1$, there is a coincidence of certain levels across the three columns.

$= 0, 1, 2, \ldots$, the values of μ_n and ν_n and, for later purposes, the value of $\mu_n + \nu_n - 2n$. The eigenvalue spectrum can be compared with that of a harmonic oscillator of frequency ω_2 and of frequency ω_1 as shown in Fig. 1. On the left is the spectrum for a *harmonic* oscillator of frequency ω_2, and on the right that of frequency ω_1. The center spectrum is for the *biharmonic* oscillator with these frequencies. As is evident from the figure, the *biharmonic* oscillator levels are nearly equally spaced.

In Table II and Fig. 2, we show the same kind of information for $\omega_2 = 5\omega_1$. Again the energy levels are almost equally spaced. An interesting feature occurs for this frequency ratio of 5:1. Certain *biharmonic* oscillator levels coincide exactly with appropriate levels of the respective *harmonic* oscillators. This occurs only when the frequencies are in the ratio of two odd integers and corresponds to *integer* root values for μ and ν such that

$$(\mu + \tfrac{1}{2})\omega_1 = (\nu + \tfrac{1}{2})\omega_2$$

or

$$\omega_2/\omega_1 = (2\mu + 1)/(2\nu + 1),$$

and Eq. (7) is satisfied by having both tangent functions (or their reciprocals) vanishing.

Wave functions for the biharmonic oscillator have just the appearance one would expect for an asymmetric potential well. In Figs. 3 and 4 are shown respectively, the ground state and sixth excited state wave functions for a frequency ratio of 5:1. Also superimposed in each of these drawings is a plot of the potential energy function.

We return now to the observation that the energy levels for the *biharmonic* oscillator are very nearly equally spaced for any frequency ratio. This result is reflected in Tables I and II in the approximate equality, $\mu_n + \nu_n \approx 2n$, $n = 0, 1, 2, \ldots$. To see this, we write

$$\mu_n + \nu_n = 2(n + \Delta_n),$$

with Δ_n indicating the necessary correction term, assumed to be small. In addition, we have

$$E_n = (\mu_n + \tfrac{1}{2})\hbar\omega_1 = (\nu_n + \tfrac{1}{2})\hbar\omega_2,$$

and these two equations can be solved for μ_n and ν_n. The result for the energy eigenvalue of the state labeled by n is

$$E_n = (n + \tfrac{1}{2} + \Delta_n)\hbar 2\omega_1\omega_2/(\omega_1 + \omega_2). \tag{9}$$

To the extent then that Δ_n can be neglected, the level spacing is the same as that of a *harmonic* oscillator of frequency $\omega = 2\omega_1\omega_2/(\omega_1 + \omega_2)$.

It is not obvious at this point, however, that Δ_n must be small. The result follows from the eigenvalue root equation, Eq. (7), and an interesting property of the gamma function ratios in that expression. Again we write for the state labeled by n,

$$\mu_n + \nu_n = 2(n + \Delta_n),$$

or

$$\nu_n = 2(n + \Delta_n) - \mu_n.$$

Then, in Eq. (7),

$$\tan(\pi\nu_n/2) = -\tan(\pi\mu_n/2 - \pi\Delta_n).$$

Table II. Energy level parameters for $\omega_2 = 5\omega_1$.

n	μ_n	ν_n	$\mu_n + \nu_n - 2n$
0	0.4053	−0.3189	0.0864
1	2.0000	0.0000	0.0000
2	3.6536	0.3307	−0.0157
3	5.3257	0.6651	−0.0092
4	7.0000	1.0000	0.0000
5	8.6702	1.3340	0.0042
6	10.3360	1.6672	0.0032
7	12.0000	2.0000	0.0000

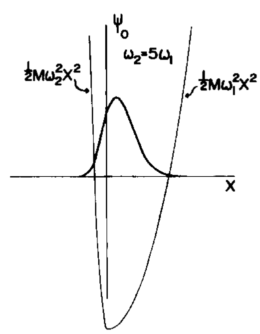

Fig. 3. The ground state biharmonic oscillator wave function is shown for $\omega_2 = 5\omega_1$. Also shown is the potential energy function arbitrarily displaced downward.

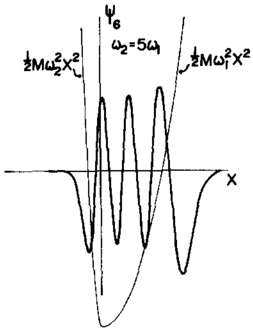

Fig. 4. The sixth excited state wave function of the biharmonic oscillator is shown for $\omega_2 = 5\omega_1$. Also shown is the potential energy function arbitrarily displaced downward.

Also,

$$\Gamma(1+\mu_n/2)=\Gamma[\tfrac{3}{4}+(\mu_n+\tfrac{1}{2})/2],$$
$$\Gamma(\tfrac{1}{2}+\mu_n/2)=\Gamma[\tfrac{1}{4}+(\mu_n+\tfrac{1}{2})/2],$$
$$\Gamma(1+\nu_n/2)=\Gamma[\tfrac{3}{4}+(\nu_n+\tfrac{1}{2})/2],$$
$$\Gamma(\tfrac{1}{2}+\nu_n/2)=\Gamma[\tfrac{1}{4}+(\nu_n+\tfrac{1}{2})/2].$$

Equation (7) can now be rewritten as

$$\tan\left(\frac{\pi\mu_n}{2}\right)=\frac{\Gamma[\frac{3}{4}+(\nu_n+\frac{1}{2})/2]\Gamma[\frac{1}{4}+(\mu_n+\frac{1}{2})/2]}{\Gamma[\frac{1}{4}+(\nu_n+\frac{1}{2})/2]\Gamma[\frac{3}{4}+(\mu_n+\frac{1}{2})/2]}\times\left(\frac{\omega_2}{\omega_1}\right)^{1/2}\tan\left(\frac{\pi\mu_n}{2}-\pi\Delta_n\right). \qquad (10)$$

The ratios of gamma functions in the above expression are of the form,

$$\Gamma(\tfrac{3}{4}+z)/\Gamma(\tfrac{1}{4}+z).$$

If z is large, an asymptotic expression for this ratio can be developed from Eq. (8). To terms of order z^{-6},

$$\Gamma(\tfrac{3}{4}+z)/\Gamma(\tfrac{1}{4}+z)=(z)^{1/2}\exp(z^{-2}/64-19z^{-4}/8192+\cdots).$$

In fact, calculation shows that this ratio of gamma functions differs from $z^{1/2}$ by 1% or less for z as small as 1.2 and by less than 5% for $z = 0.5$.

Applying this expression to order z^{-2} to the ratios in Eq. (10), we obtain

$$\tan(\pi\mu_n/2)=[(\nu_n+\tfrac{1}{2})\omega_2/(\mu_n+\tfrac{1}{2})\omega_1]^{1/2}\times\exp\{[(\nu_n+\tfrac{1}{2})^2-(\mu_n+\tfrac{1}{2})^2]/16\}\times\tan(\pi\mu_n/2-\pi\Delta_n). \qquad (11)$$

The first factor on the right-hand side of Eq. (11) is unity since $(\nu_n + \frac{1}{2})\omega_2 = E_n/\hbar = (\mu_n + \frac{1}{2})\omega_1$. So, for sufficiently large values of μ_n and ν_n, Δ_n is very small. A first-order expression for Δ_n obtained from Eq. (11) is

$$\pi\Delta_n\approx\omega_1^{-2}(\omega_2^2-\omega_1^2)\frac{\tan(\pi\mu_n/2)}{(\mu_n+\frac{1}{2})^2},$$

for μ_n not close to an odd integer. The sign of Δ_n is then the same as that of the tangent function, $\tan(\pi\mu_n/2)$, as inspection of Tables I and II shows.

The above analysis is based on the use of asymptotic expansions, that is, μ_n and ν_n (or n) large. They appear to be valid, however, even for $n = 1$ for reasonable frequency ratios.

Another indication of nearly equally spaced levels can be obtained by applying the Bohr–Sommerfeld quantization rule to the biharmonic oscillator. The evaluation of the integral

$$\oint p\,dx=nh,$$

is straightforward and leads to the uniformly spaced spectrum,

$$E_n=n\hbar 2\omega_1\omega_2/(\omega_1+\omega_2),$$

which should be compared with Eq. (9).

An interesting sidelight of the biharmonic oscillator model deals with the familiar Einstein model of the lattice contribution to the specific heat capacity of a solid. The Einstein model is usually invoked after the harmonic approximation has been made; that is, a collection of *harmonic* oscillators of frequency ω is considered. All that is needed for the calculation, however, is the equal spacing of oscillator energy levels. One can also consider a collection of *biharmonic* oscillators with frequencies ω_1 and ω_2. To the extent that the Δ_n can be neglected, the biharmonic energy levels are given by

$$E_n=(n+\tfrac{1}{2})\hbar\omega,\quad n=0,1,2,\ldots,$$

with $\omega = 2\omega_1\omega_2/(\omega_1 + \omega_2)$, and the partition sum,

$$\sum_n\exp(-\beta E_n),$$

can be evaluated. Thus the success of the Einstein model is not necessarily connected with the validity of the harmonic approximation.

Other features of the biharmonic oscillator model can be developed. For example, matrix elements of interest can be evaluated numerically; dipole selection rules are different from those of the harmonic oscillator; perturbation schemes may be considered. The biharmonic oscillator may then be a valuable addition to the collection of exactly solvable models for quantum-mechanical systems.

[1]H. W. Graben and W. Edward Gettys (unpublished).

[2]*Higher Transcendental Functions*, edited by A. Erdelyi (McGraw-Hill, New York, 1953), Vol. I.

[3]The parabolic cylinder function has been used in the treatment of the double oscillator; see E. Merzbacher, *Quantum Mechanics* (Wiley, New York, 1970), 2nd ed.