Pseudoharmonic Oscillators and Inadequacy of Semiclassical Quantization

Frank H. Stillinger* and **Dorothea K. Stillinger**[†]

AT&T Bell Laboratories, Murray Hill, New Jersey 07974 *(Received: February 1, 1989; In Final Form: May 22, 1989)*

The condition on a one-dimensional potential that all its classical trajectories be bounded and possess an energy-independent period includes, but is not restricted to, harmonic oscillators. We have explicitly constructed a parametric set of "pseudoharmonic oscillators" with this property. The corresponding potentials $V(x)$ are analytic along the entire real x axis, and are displayed in closed form. The Einstein–Brillouin–Keller prescription for zeroth-order semiclassical quantization leads to the familiar harmonic oscillator spectrum for all of these pseudoharmonic oscillators. Exact Schrödinger-equation eigenvalues have also been obtained for a limiting case, the split harmonic oscillator (unequal left and right side harmonic forces). Consequently one sees that the uncorrected semiclassical approximation applied to pseudoharmonic oscillators misses several significant qualitative features of the exact spectrum.

Introduction

Harmonic oscillators have the well-known property that all classical trajectories are periodic and that the oscillation period is independent of total energy. This property is not unique to harmonic oscillators but extends to a family of "pseudoharmonic oscillators" which form the subject of this report. Some of these have been considered before,[1,2] including the harmonic oscillator with centripetal barrier.[3] However, we will exhibit below, apparently for the first time, a parametric set of pseudoharmonic oscillator potentials in closed form that are analytic over the entire real line.

Nieto and Gutschick[3] have demonstrated that quantum oscillators with equally spaced energy levels can have nonharmonic classical dynamics (i.e., oscillation period varying with energy). They have also raised the reverse question of whether a classical pseudoharmonic oscillator, when quantized, could display unequal energy level spacings. Using our specific set of examples we are able to answer this question in the affirmative, in spite of the contrary conclusion offered by leading-order semiclassical quantization.

Analytic Set of Pseudoharmonic Oscillators

Let $V(x)$ be a continuous and differentiable potential function defined on the real x axis, with the following conditions: (a) $V(0) = 0$, (b) $(\mathrm{sgn}\ x)V'(x) > 0$ for $|x| > 0$, (c) $V(x) \to +\infty$ as $|x| \to \infty$. These guarantee that all classical trajectories are periodic and pass through $x = 0$.

Inverting $V(x)$ leads to two branches $x_-(V) \leq 0$ and $x_+(V) \geq 0$ defined for $V \geq 0$. By requiring

$$x'_+(V) - x'_-(V) = (2/KV)^{1/2} \tag{1}$$

we ensure that all trajectories have the same energy-independent oscillation period as if the potential were that for the harmonic oscillator $\frac{1}{2}Kx^2$. The interpretation of eq 1 is elementary: time increments spent by the oscillator in passing between V and $V + dV$ respectively for $x < 0$ and for $x > 0$ deviate from harmonic oscillator values in exactly compensating ways. Equation 1 can be satisfied by choosing

$$x_\pm(V) = \pm(2V/K)^{1/2} + g(V) \tag{2}$$

provided the resulting $V(x)$ is single-valued on the real axis and meets conditions a–c above.

A wide range of functions $g(V)$ is available to generate pseudoharmonic oscillators. For concreteness consider the case

$$g(V) = \xi\beta^{-1/2}[(1 + 2\beta V/K)^{1/2} - 1] \tag{3}$$

where $|\xi| < 1$ and $\beta > 0$ but are otherwise arbitrary parameters.

† Resident visitor.

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With this choice eq 2 can be explicitly inverted to give a pseudoharmonic oscillator potential that is free of singularities along the entire x axis:

$$V(x) = \tfrac{1}{2}K(1 - \xi^2)^{-2}\{x + \xi\beta^{-1/2}[1 - (1 + 2\xi\beta^{1/2}x + \beta x^2)^{1/2}]\}^2 \quad (4)$$

$$= \tfrac{1}{2}K[x^2 - \xi\beta^{1/2}x^3 + O(x^4)]$$

In the limit that β becomes infinite this reduces to a "split harmonic oscillator" potential:

$$\lim_{\beta\to\infty} V(x) = \tfrac{1}{2}K(1 - \xi)^{-2}x^2 \qquad (x < 0)$$

$$= \tfrac{1}{2}K(1 + \xi)^{-2}x^2 \qquad (x > 0) \quad (5)$$

Conventional harmonic oscillator behavior is recovered as β approaches 0 for any ξ.

Semiclassical quantization has been a popular approach to explaining spectra of simple dynamical systems for which action-angle variables can be defined.[4] Extensions have also been suggested to cover cases with coupled degrees of freedom for which sufficiently regular classical trajectories existed.[5,6] These extensions have had numerous useful applications to problems in chemical physics.[7,8]

The Einstein–Brillouin–Keller semiclassical quantization rule for a one-dimensional oscillator is[9–11]

$$J = \oint p\,dq = (n + \tfrac{1}{2})h \qquad (n = 0, 1, 2, ...) \quad (6)$$

where p and q are conjugate momentum and coordinate variables, h is Planck's constant, and the action integral spans one period of motion. As is well-known, this rule reproduces the exact energy eigenvalues for the harmonic oscillator.

In the case of our pseudoharmonic oscillator set eq 4, the action integral in eq 6 can be transformed into a sum of integrals over potential V between limits 0 and E, the total energy. Subsequent appeal to eq 1 then easily leads to the result

$$J(E) = 2\pi E/\omega \quad (7)$$

where ω is the energy-independent angular frequency

$$\omega = (K/m)^{1/2} \quad (8)$$

and m is the oscillator mass. Expression 7 is identical in form with that for harmonic oscillators. Consequently the Einstein–Brillouin–Keller rule leads to an eigenvalue spectrum for pseudoharmonic oscillators

$$E_n = (n + \tfrac{1}{2})\hbar\omega \quad (9)$$

which is identical with the harmonic counterpart. Note that nonuniqueness of $V(x)$ given semiclassical E_n's is well-known from one-dimensional RKR inversion.[8]

Energy Eigenvalues

Energy eigenvalues obtained from the full quantum mechanical treatment of the pseudoharmonic set (4) are expected to be continuous functions of the anharmonicity parameters ξ and β. Therefore any discrepancy between such a treatment and the semiclassical prediction (9) that appears in, say, the split harmonic oscillator limit $\beta \to \infty$ would also obtain for some range of finite β.

The exact eigenfunctions for the split harmonic oscillator defined in eq 5 above consist of parabolic cylinder functions[12] with separate

TABLE I: Coefficients for Second-Order Dependence of Split Harmonic-Oscillator Eigenvalues on the Anharmonicity Parameter ξ [Eq 11]

n	c_n
0	(1/4)(1 − ln 2) = +0.0767132...
1	(3/4)(2 − 3 ln 2) = −0.0595811...
2	(5/8)(7 − 10 ln 2) = +0.0428301...
3	(7/24)(29 − 42 ln 2) = −0.0327196...
4	(9/16)(25 − 36 ln 2) = +0.0262695...
5	(11/240)(457 − 660 ln 2) = −0.0218688...

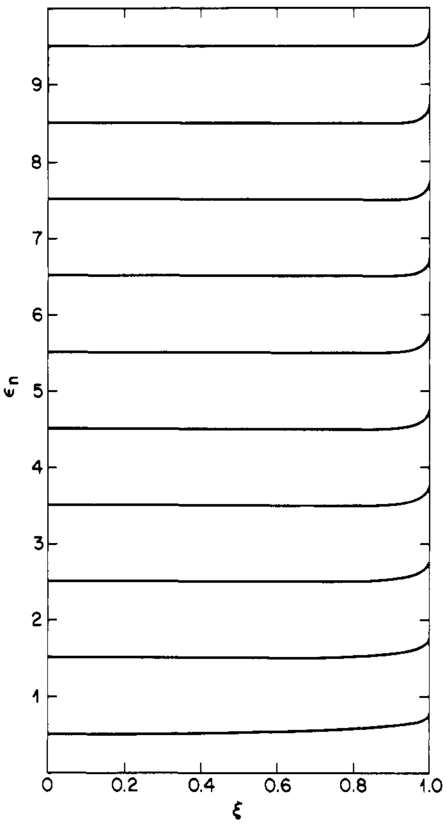

Figure 1. Dependence of split harmonic oscillator eigenvalues on the anharmonicity parameter ξ. Each ϵ_n is an even function of ξ.

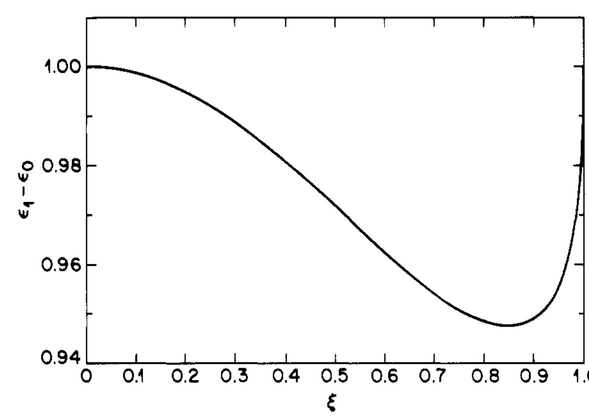

Figure 2. Difference between the two lowest eigenvalues as a function of the anharmonicity parameter ξ. The semiclassical approximation predicts that this difference is identically 1.

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variables for positive and for negative x. By imposing continuity on eigenfunctions and their first derivatives at $x = 0$ one derives the following transcendental equation for determination of the $\epsilon_n \equiv E_n/\hbar\omega$:

$$\frac{\Gamma\left[\frac{3}{4} - \frac{1}{2}(1+\xi)\epsilon_n\right]}{\Gamma\left[\frac{3}{4} - \frac{1}{2}(1-\xi)\epsilon_n\right]} + \frac{(1+\xi)^{1/2}\Gamma\left[\frac{1}{4} - \frac{1}{2}(1+\xi)\epsilon_n\right]}{(1-\xi)^{1/2}\Gamma\left[\frac{1}{4} - \frac{1}{2}(1-\xi)\epsilon_n\right]} = 0 \quad (10)$$

It is clear that the ϵ_n must be even functions of ξ; changing the sign of ξ is equivalent to switching sides of the split harmonic oscillator, and it merely interchanges numerators and denominators in eq 10.

By using standard properties of the Γ function[13] it is possible to extract the small-ξ behavior of the ϵ_n:

$$\epsilon_n(\xi) = n + \tfrac{1}{2} + c_n\xi^2 + O(\xi^4) \quad (11)$$

Explicit values for the first few coefficients c_n are displayed in Table I. The striking feature of these results is that they alternate in sign, revealing an initial tendency as ξ moves from zero for neighboring eigenvalues to pair (though this effect appears to diminish with increasing quantum number n). This indicates a deviation from the semiclassical prediction.

We have also carried out a numerical analysis of eq 10 to trace out the full ξ dependence of the ϵ_n. Figures 1 and 2 exhibit some results. The unequal level spacings initially detected by eq 11 persist until $|\xi|$ reaches +1, at which point the eigenvalues are

$$\epsilon_n(|\xi| = 1) = n + \tfrac{3}{4} \quad (12)$$

In this limit one half of the split harmonic oscillator has become an impenetrable wall, and the eigenstates confined to the other half correspond to the odd subset for the $\xi = 0$ harmonic oscillator, suitably rescaled.

The $\epsilon_n(\xi)$ curves in Figure 1 have several notable features. Most obvious is the infinite slope that develops as $\xi \to 1$. From eq 10 it is possible to show that a square-root singularity is involved:

$$\epsilon_n(\xi) = n + \tfrac{3}{4} - d_n(1-\xi)^{1/2} + O(1-\xi)$$

$$d_n = \left[\Gamma\left(\frac{1}{4}\right)/2\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{3}{4}\right)\right]\prod_{j=1}^{n}(1 + 1/2j) \quad (13)$$

Notice that the strength of this singularity increases logarithmically with n.

With the exception of the ground state, none of the $\epsilon_n(\xi)$ curves is monotonic over $0 \le \xi \le 1$. Instead an oscillatory behavior develops with increasing n, the amplitude of which is largest near $\xi = 1$. This characteristic is illustrated by Figure 3. Our numerical results suggest that $\epsilon_n(\xi)$ possesses n relative maxima and minima in $0 < \xi < 1$.

(13) Reference 12, Chapter 6.

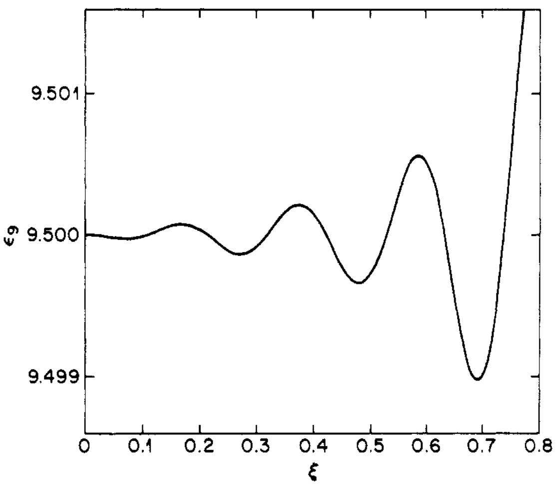

Figure 3. Vertically expanded view of a portion of the $\epsilon_9(\xi)$ curve, illustrating the damped oscillatory behavior occurring for the larger quantum numbers.

The flattening that develops with increasing n in the $\epsilon_n(\xi)$ curves for most of the ξ range confirms the belief that the semiclassical quantization method should become more nearly exact the higher the energy. However, the behavior is obviously nonuniform in ξ, with the steep-walled limits $|\xi| = 1$ continuing to resist the uncorrected semiclassical description, eq 9.

We note in passing that the *classical* partition functions (canonical or microcanonical) for pseudoharmonic oscillators are identical with those for the corresponding harmonic oscillators.[14]

Conclusion

Our results for pseudoharmonic oscillators stress the need for caution in applying semiclassical quantization to problems of physical interest. Subtle features of the eigenvalue spectrum are missed by the semiclassical approach for the example investigated here, and there is the possibility of analogous imprecision in more complicated cases. Some engaging questions also arise from the present work about coherent states for pseudoharmonic oscillators that would be defined by the Nieto and Simmons approach,[15] which generalizes the well-known formalism for harmonic oscillator coherent states.[16] Finally, we have the open question whether in any nontrivial sense pseudoharmonic potentials can exist in two or more dimensions, and if they do, whether their quantum dynamics can be chaotic.[17]

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