Harmonic? Anharmonic? Inharmonic?

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In molecular spectroscopy, an anharmonic oscillator has a nonparabolic potential which results in a nonharmonic absorption spectrum, but the same oscillator treated classically has a precisely harmonic vibrational spectrum. To avoid confusion, it is suggested that such an oscillator should simply be called nonlinear. The term ''inharmonic'' is suggested as an appropriate descriptor for classical oscillators, such as metal bars, that have nonharmonic vibrational spectra even in the linear limit of small vibrations.
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I. INTRODUCTION

This paper was provoked by the response of a colleague, working in the field of atomic and molecular physics, to the author's use of the word ''inharmonic'' to describe the overtones in the sound of a bell. Why not, he asked, use the common term ''anharmonic''? An explanation perhaps convinced him of the difference between the two terms and was the subject of a brief Letter to the Editor of the Australian journal *The Physicist*.[1] However, because the confusion of terminology seems to be widespread, the matter is perhaps worthy of a more detailed exposition.

II. SIMPLE HARMONIC OSCILLATORS

Everyone who teaches physics is familiar with the term ''simple harmonic oscillator.'' Briefly, it refers to a dynamical system with a single degree of freedom and a linear restoring force, as expressed by the differential equation

$$m\frac{d^2z}{dt^2}=-K(z-z_0), \tag{1}$$

where z is the displacement coordinate, z_0 is the equilibrium position, t is time, m is the mass of the moving particle, and K is the restoring force constant. A term describing damping could be added, but it is unnecessary in the context of the present discussion. The solution, of course, is

$$z(t)=z_0+A\sin(\omega t+\phi), \tag{2}$$

where

$$\omega=(K/m)^{1/2}, \tag{3}$$

A is the vibration amplitude, and ϕ is a phase constant. This oscillator can also be considered as a particle moving in a parabolic potential well $V=K(z-z_0)^2/2$.

The only mystery is why such an oscillator should be called ''harmonic.'' A harmonic series is well known in mathematics and is the set $\{a_n\}$ with $a_n=1/n$. The relation to music has been well established since the time of Pythagoras, when pleasant sounds were found to result from plucking strings with lengths in the ratio of simple integers.[2] In a more modern context, complex tones with upper partials (that is, Fourier components of frequency higher than the fundamental) whose frequencies are exact integer multiples of the frequency of the fundamental are commonly produced by sustained-tone musical instruments,[3] and these upper partials are called ''harmonics.''[4]

Here we have a system with just one frequency—why should it be called harmonic? Perhaps melodic would be a better term. The added descriptor ''simple'' appears to be apt, but it implies the existence of a ''complex harmonic oscillator'' or something of the sort, and that designation does not appear to have been used.

III. NONLINEAR OSCILLATORS

The word ''anharmonic'' appears in atomic and molecular physics to describe a nonlinear oscillator whose behavior is described by

$$m\frac{d^2z}{dt^2}=-f(z-z_0), \tag{4}$$

where the force $f(z)$ is a nonlinear function of z, though usually with a dominant first-order term at the amplitudes considered. The potential well $V(z)$ is then a distorted parabola centered on z_0. A typical example is the potential between the two components of a diatomic molecule, which has the approximate form[5]

$$V(r)=ar^{-m}-br^{-n}, \tag{5}$$

where r is the interatomic spacing, and a and b are positive numbers. The particular case of the Lennard-Jones potential has $m=12$ and $n=6$.

The behavior of such a system has been thoroughly studied, not just as an isolated oscillator, but also as a driven oscillator with dissipation, in which case the behavior can be truly complex and indeed chaotic.[6,7] These complexities are not of concern here, but rather simply the behavior of the one-degree-of-freedom system described by Eq. (4). Because the total energy E of the system is conserved, the particle velocity is a simple function of position

$$\frac{dz}{dt}=\pm\left[\frac{2E}{m}-\frac{2}{m}\int_0^z f(\zeta-z_0)\,d\zeta\right]^{1/2}, \tag{6}$$

and the particle's behavior is therefore a simple repetitive oscillation. Such an oscillation can be analyzed into its Fourier components, and these turn out to have frequencies that are exact integer multiples of the fundamental frequency—they are exact harmonics of the fundamental.

An extreme example of such a nonlinear oscillator is the simple case of a particle in a one-dimensional box potential, $V(z)=0$ for $-a<z<a$ and $V(z)=\infty$ for $|z|\geqslant a$. If the particle mass is m and its energy is E, then the fundamental oscillation frequency is

$$\omega_1=\frac{\pi}{2a}\left(\frac{2E}{m}\right)^{1/2}. \tag{7}$$

Plotted against time, the displacement follows a square-wave pattern, and the frequency spectrum is precisely harmonic, with amplitudes $A_n=4a/\pi n$ for n odd and zero for n even.

A reasonable terminology would be to refer to such a system as a ''complex harmonic oscillator,'' or just a ''harmonic oscillator,'' or certainly a ''nonlinear oscillator,'' but some physicists have chosen instead the apparently inappropriate term ''anharmonic oscillator,'' incorrectly implying by this name that the overtone frequencies, or upper partials, are not harmonics, because the prefix ''an'' implies negation.

Nonlinear oscillators are common in areas other than atomic and molecular physics, and indeed are at the heart of the process of sound generation in sustained-tone musical instruments such as violins, clarinets, and trumpets,[3] where they are responsible for the generation of the rich harmonic sounds of these instruments. The fact that sustained-tone instruments produce sounds with harmonic overtones is, in turn, responsible for the structure of Western music, its scales, concords, and discords.[8]

Returning to the question of nomenclature, we find the origin of the term ''anharmonic'' in the infrared spectra of diatomic molecules.[9,10] A simple harmonic oscillator with a parabolic potential has, in quantum mechanics, the series of energy levels $E_n=(n+\frac{1}{2})\hbar\omega$, where ω is the classical frequency given by Eq. (3). The quantum selection rules in this case dictate that transitions can occur only between levels n and $n\pm 1$ so that only a single vibrational absorption line would be observed. The spectrum is, of course, complicated by the presence of rotational levels. When the restoring force is nonlinear, as it always is in reality, the energy levels can be written as[9,10]

$$E_n=(n+\tfrac{1}{2})\hbar\omega[1-A_1(n+\tfrac{1}{2})+A_2(n+\tfrac{1}{2})^2+\cdots], \tag{8}$$

where A_1 is the first anharmonicity constant, A_2 is the second anharmonicity constant, and so on.

Because of the asymmetry of the interatomic potential, transitions between levels n and $n\pm m$ are allowed for values of m greater than unity, although these transitions appear at much lower intensity in the spectrum than does the fundamental absorption transition $n=0\rightarrow n=1$. Although the absorption spectrum is complicated by rotational transitions, the vibrational transitions define a sequence of overtone bands,[9,10] the infrared frequencies of which are not exact integer multiples of the fundamental frequency.

This lack of harmonic relationship between the frequencies of the overtone bands is the origin of the term anharmonic in molecular spectroscopy. Although it is certainly appropriate to describe the absorption spectrum of a diatomic molecule as anharmonic, we see that this inharmonicity is related to changes in the oscillator frequency with vibration amplitude, and not to any lack of harmonicity in the classical oscillator spectrum.

IV. INHARMONIC OSCILLATORS

There is a third important class of oscillators that is distinguished by the fact that its overtones are not harmonics of the fundamental, and we refer to these as ''inharmonic oscillators.'' A formal example is the oscillator described by the fourth-order linear partial differential equation

$$\frac{\partial^2 z}{\partial t^2}=S\frac{\partial^4 z}{\partial x^4}, \tag{9}$$

which describes the oscillations of an elastic beam.[4] Here z is the displacement coordinate, x is the coordinate along the length of the beam, and S is the beam stiffness divided by its mass. If the beam is assumed to either have free ends or else to have both ends rigidly clamped, then its mode frequencies are approximately $\omega_n\approx C(n+\frac{1}{2})^2$, where C is a constant.[4] These frequencies are clearly not in harmonic relationship, so that the term inharmonic is appropriate.

The elastic beam is but one example of this type of oscillator, and indeed essentially all idiophones, by which is meant sound-producing instruments that do so by virtue of their own vibration, such as gongs and bells, are inharmonic. The only partial exception is the bells of Western carillons, which have been shaped and tuned so that their first few mode frequencies are in nearly integer relationship. The sounds of inharmonic oscillators are common in Asian music based on gongs, an example being the Indonesian Gamelan orchestra. The scales and harmonies used differ considerably from those of Western music based upon sustained-tone harmonic oscillators, but are in fact equally pleasant. A detailed analysis of scales and harmonies based upon inharmonic sounds has been given by Sethares.[11]

V. CONCLUSIONS

It would be impractical to suggest abandonment of the term simple harmonic oscillator, because it has been embedded in the literature for more than a century. The adjective anharmonic, when applied to molecular absorption bands, would be similarly difficult to change, though I would urge spectroscopists to refer to an ''anharmonic spectrum'' rather than to characterize the oscillator itself as anharmonic and refer instead to the oscillator as simply nonlinear. In other fields of physics involving vibration, there should be a clear distinction made between nonlinear vibrators and those that are genuinely inharmonic in that they have nonharmonic mode frequencies; the term anharmonic should be studiously avoided because of the confusion it is likely to cause (though unfortunately nonlinear vibrators are called anharmonic in some very reputable physics texts).[12]

Of course, those familiar with music theory will know that there is also a term ''enharmonic''—but that is another story![13,14]

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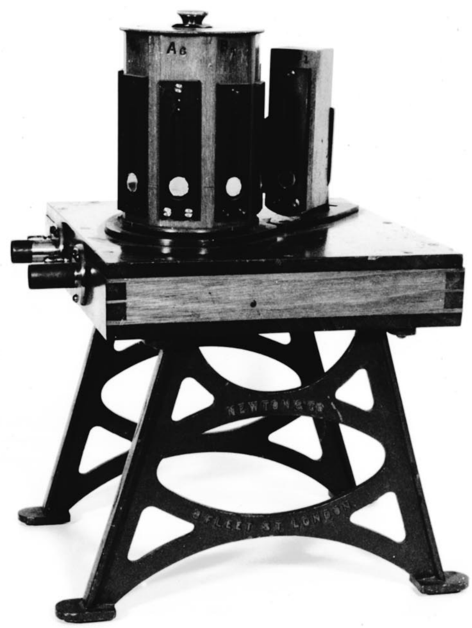
[1]N. H. Fletcher, ''Harmonic? Anharmonic? Inharmonic?,'' The Physicist **37**, 189 (2000).

[2]F. V. Hunt, *Origins in Acoustics* (1978) (reprinted by Acoustical Society of America, Woodbury, NY, 1992), Chap. 1.

[3]N. H. Fletcher, ‘‘The nonlinear physics of musical instruments,’’ Rep. Prog. Phys. **62**, 723–764 (1999).
[4]P. M. Morse, *Vibration and Sound* (1948), 2nd ed. (reprinted by Acoustical Society of America, Woodbury, NY, 1981), pp. 85, 161–162.
[5]J. Goodisman, *Diatomic Interaction Potential Theory* (Academic, New York, 1973), Vol. 1, pp. 72–86.
[6]*Universality in Chaos*, edited by P. Cvitanovic (Adam Hilger, Bristol, 1984).
[7]G. L. Baker and J. P. Gollub, *Chaotic Dynamics: An Introduction* (Cambridge U.P., Cambridge, 1996).
[8]H. L. F. Helmholtz, *On the Sensations of Tone* (1877), 4th ed., translated by A. J. Ellis (Dover, New York, 1954).
[9]G. Herzberg, *Molecular Spectra and Molecular Structure* (Van Nostrand, New York, 1950), pp. 90–92.
[10]M. D. Harmony, ‘‘Molecular spectra and structure,’’ in *A Physicist's Desk Reference*, edited by H. L. Anderson (American Institute of Physics, New York, 1989), p. 242.
[11]W. A. Sethares, *Tuning, Timbre, Spectrum, Scale* (Springer, London, 1998).
[12]A. B. Pippard, *The Physics of Vibration* (Cambridge U.P., Cambridge, 1978), Vol. 1, pp. 12–21.
[13]In music theory an enharmonic change is one in which the naming of a note changes, for example, from G♯ to A♭. In modern equal-tempered tuning, as for example on the piano, there is no pitch change involved, but in older and more subtle tuning systems, such as meantone (Ref. 14) there is a pitch change of a small fraction of a semitone.
[14]J. Backus, *The Acoustical Foundations of Music* (W. W. Norton, New York, 1969), Chap. 8.



Tune Analyzer. This apparatus uses Lissajous figures to show that the ratio of the frequencies in a diatonic scale are ratios of small numbers. On the right-hand side is an air-driven vibrating reed (a harmonica reed) with a small mirror attached to its free end. The revolving drum contains eight reeds, ranging up the scale from the same frequency as the fixed reed to its octave. In use, the box holding the fixed reed would be rotated 90 degrees, making it oscillate at right angles to the other reeds. A beam of light reflecting from the two reeds in succession undergoes simple harmonic motion in two perpendicular directions, thus producing a Lissajous figure. The shape of the figures produced by two frequencies which bear small number ratios to each other is well-known. The apparatus, by Newton and Company of London, dates from the last quarter of the nineteenth century, and is in the collection of the Smithsonian Institution. (Photograph and notes by Thomas B. Greenslade, Jr., Kenyon College)