Orbital Shaped Standing Waves Using Chladni Platess

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Abstract: Chemistry students are often introduced to the concept of atomic orbitals with a representation of a one-dimensional standing wave. The classic example is the harmonic frequencies, which produce standing waves on a guitar string; a concept that is easily replicated in class with a length of rope. From here, students are typically exposed to a more realistic three-dimensional model, which can often be difficult to visualize. Extrapolation from a two-dimensional model, such as the vibrational modes of a drumhead, can be used to convey the standing wave concept to students more easily. We have opted to use Chladni plates, which may be tuned to give a two-dimensional standing wave that serves as a cross-sectional representation of atomic orbitals. The demonstration, intended for first year chemistry students, facilitates the examination of nodal and anti-nodal regions of a Chladni figure that students can connect to the concept of quantum mechanical parameters and their relationship to atomic orbital shape.

Introduction

Understanding that an electron in an orbital can be thought of as a three-dimensional standing wave is a tough concept to wrap one's head around. A one dimensional standing wave is easy to visualize and demonstrate in a lecture environment - a length of rope held at each end by volunteers can be induced into a standing wave, which if energetic enough, will readily display nodes [1, 2]. However, making the jump to a three-dimensional wave is much tougher, perhaps because our minds run out of dimensions to consider. Length, breadth, and depth are conceivable; but where does the amplitude go? The meanings of the different regions of the wave can be even more confusing given the multi-dimensionality of the problem. If we back off one dimension, and consider a two-dimensional standing wave, it becomes easier - we can use the third dimension to convey the amplitude, and the standing waves, if chosen carefully, can illustrate the cross-sectional shape of the orbital. A physical demonstration of wave behaviour in two dimensions, prior to three-dimensional illustration through computer-based models, allows for direct student involvement and easier conceptualization of a complex problem in first-year Chemistry.

The shape of orbitals has been taught to students using media as diverse as circular magnets [3], Styrofoam models [4, 5], beakers of coloured water [6], computer-generated images [7], and balloons [8]. Various simple models have been used to introduce the concept of standing waves to students in the context of atomic (and/or molecular) orbitals. Instructors have tapped the rim of a coffee cup to relate nodes to the energies of aromatic molecular orbitals [9], have used Kundt's tubes (devices that set up acoustic standing waves in different gaseous media as a characterization tool) [10], and have reproduced Wiener's historic experiment on a standing light wave [11] using a laser pointer [12]. Computer-based orbital illustrations are an extremely valuable advance, allowing direct visualization of the quantum mechanical solutions for atomic orbitals. There exist excellent examples in the literature of two- and three-dimensional visualizations of atomic orbitals, making use of custom or proprietary software in order to produce plots of atomic and molecular orbitals and examine the orbital's shape based on a given change in parameters [13–20].

Understanding and correctly interpreting these illustrations has become a fundamental learning goal in introductory quantum atomic structure. However, orbital shapes can be conceptually disconnected from the ideas of wave behavior in quantum chemistry. Demonstrations of wave mechanics, preferably with direct student involvement, are an effective way to illustrate and promote the correct conceptualization of wavefunction shapes, their properties and the quantum mechanical wave equation [21–23]. An appealing and effective way to perform this illustration is by using the Chladni experiment discussed in the following pages. It should be noted here that the two-dimensional acoustic waves that produce Chladni patterns have been used previously to illustrate theoretically wave behaviour: The two-dimensional wave equation is discussed at some length in Donald McQuarrie's standard textbook "Quantum Chemistry" [22] and pictures of a drum with low-frequency Chladni patterns are included. A series of analogies including Chladni patterns, jellyfish and viscous glop are used in a fascinating account of quantum chemical equivalencies by Dylan Jayatilaka from the University of Southern Australia [24]. The purpose of the current article is to illustrate how Chladni patterns can be used to physically and interactively demonstrate wave behaviour in the first-year Chemistry class.

A two-dimensional standing wave can be generated using common percussion instruments. When the appropriate harmonic frequency is applied to a drumhead the wave pattern remains in one position as the amplitude of the wave fluctuates. Above the fundamental harmonic frequency (first harmonic), the drumhead becomes segmented by nodal lines in which there is no change in amplitude; conversely, in between these nodal lines are antinodes where the change in amplitude is at a maximum [25, 26]. The standing wave formed on a drumhead is a useful analogy; however, these waves are not detectable to the unassisted naked eye, and we can more easily control and visualize two-dimensional standing waves using devices known as Chladni plates. Ernst Chladni (1756–1827) was a German physicist and musician most well-known for his study of vibrational modes produced on metal plates. In Chladni's experiment, excitation was achieved by drawing the bow of a violin across the edge of the plate. Sprinkling sand across the surface of the plate while doing so caused the sand to settle in specific patterns shaped by the nodal regions of the vibrational mode, now referred to as Chladni figures. These patterns appear as the sand is tossed away from regions of the plate where a strong vibration is occurring (primarily the antinodal regions) and settles into regions where nodal lines are present. For example, a Chladni plate plays a prominent role in a striking music video involving a variety of visualized standing waves by N. J. Stanford [27]. The modern method of generating Chladni figures is achieved with a frequency generator, a voice coil and metal plate. This in-class demonstration enables students to participate in active learning by producing a tangible representation of an atomic orbital, which they can control. The process of creating these beautiful cymatic figures is an engaging way to intrigue and educate students.

Materials

The source of the excitation signal used was a Keysight (Agilent) 33522A function-generator. A custom power-amplifier, consisting of a Canakit (cat. # CK003) 10-Watt single-channel audio amplifier circuit, volume (amplitude) control and associated power-supply, was used to boost the signal to the levels required to drive the voice-coil that vibrates the plate. The voice-coil used was a PASCO SF-9324 mechanical wave driver. The function-generator was connected to the power-amplifier by a BNC cable. The power-amplifier positive and negative outputs were connected to the voice-coil by banana-connector cables. The aluminum plates used were round (24 cm diameter) or square (24×24 cm) and 1 mm thick. The plates were anchored to the voice-coil at their centre. ACS reagent grade sodium bicarbonate powder was purchased from EMD Chemicals and was used as the visualization medium. Other light, non-hygroscopic powders would work equally well.

Procedure

A thin layer of sodium bicarbonate is sprinkled over the whole surface of the metal plate prior to applying a frequency. The frequency generator was set to deliver a continuous 100 mVpp sine wave (without a sound-dampening cover, less than 70 mVpp may be more suitable for higher frequency patterns and will often yield similar results), and the frequency was swept through a range of approximately 50 to 4000 Hz during a test of the apparatus. Different sized plates may produce different vibrational modes of interest at any given frequency, so a sweep from approximately 50 Hz to as high as 5 kHz (see Safety section) at a slow rate is recommended in order to observe the progression of standing wave patterns in order to find the frequencies that produce patterns of interest. For demonstration purposes, a custom software was employed to quickly recall and apply the frequency and amplitude settings that produce desired standing wave patterns.

Hazards and Safety

At higher frequencies Chladni plates can become extremely loud and high-pitched [28]. Therefore, during a demonstration it is recommended that the plates are placed within a transparent, sound-dampening box to prevent aural discomfort. When initially testing a Chladni setup, ear protection is recommended since the operator will spend considerably more time working with the setup than during the relatively short demonstration.

Sodium bicarbonate (baking soda) is generally safe to handle; however, some care must be taken to avoid inhalation or eye contact. There is an increased risk of aerosolizing fine sodium bicarbonate due to the nature of this experiment. Inhalation and exposure is not considered hazardous as baking soda is generally harmless.

Discussion

Many students struggle to imagine the wave-like properties of an electron in three dimensions; a concept which becomes crucial later in the first-year semester and beyond for topics including periodic trends, chemical bonding, and reactivity. The shapes of atomic orbitals are also critical for students to fully understand as the concept is used to expound on molecular shapes, hybridization and molecular orbitals, which necessitate a spatial understanding of atomic orbitals. The association of electronic behaviour with the concept of a standing wave can also help explain questions like "Why doesn't the electron fall into the nucleus?" [29] and "How does the 2p electron go from one side of the wavefunction through the node to the other side?" [30]. The goal of this experiment is to introduce first year chemistry students to fundamental quantum theory essential in understanding atomic orbitals by facilitating a means for students to visualize simple atomic orbitals in three-dimensions through the extrapolation of the analogous two-dimensional standing-wave system generated by means of Chladni plates (Figure 2).

Physical underpinnings of the experiment. Standing waves are produced by the interference of outgoing and incoming waves in a material, at resonance frequencies, which are device-specific. Guitar strings, for example, are anchored at both ends. Plucking the string creates a set of outgoing waves. Each of these reflects at the ends of the string into returning waves. The interference between an outgoing and a reflected wave produces a standing wave with nodes at the anchoring points, which cannot, presumably, vibrate [1]. All the harmonics have these two nodes, as well as an increasing number of nodes along the string length, for higher harmonics (see Supporting Material). The fundamental frequency of the vibration depends on the length of the string, the tension in the string, and its mass, so each of these factors can in turn be used to change the tune that is played. All the harmonics are solutions of the wave equation for the guitar string, with boundary conditions given by the requirement for nodes at the anchoring points.

A drum or stretched membrane functions in a similar way, with boundary conditions (nodes at the edge because of the attachment of the membrane) imposing the periodicity of the vibrational wave. The two-dimensional standing waves are

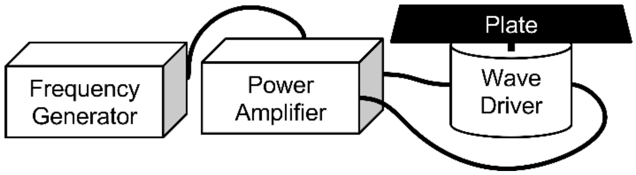

Figure 1. Schematic of the demonstration setup.

Figure 2. A Chladni figure and the corresponding visualized orbital ($6g_{z^4}$).

solution of a two-dimensional wave equation in cylindrical coordinates (for circular membranes) or Cartesian coordinates (for square membranes), and are shaped such that the width of the membrane fits multiples of half a wavelength (for pictures and animations of the square membrane vibrational modes, see the Partial Differential Equations app for Mathematica, by Dzamay, A.) [31]. Nodes on a circular membrane are diametric or circular, whereas nodes on square membranes can become significantly more complex. The free-edge Chladni apparatus used in this experiment has a distinct set of non-zero boundary conditions, based on the confinement of the wave to the size and rigidity of the plate, and the elastic behavior of the material. However, because of the principles of wave reflection and the symmetry of the problem, nodal curvatures in free-edge Chladni plates and attached-edge membranes are similar. The Chladni plate nodal planes discussed in the present work are also similar to the two-dimensional projections (which is a usual representation) of the nodal surfaces of hydrogen atomic orbitals. Parallels between the two systems can help drive home the wave nature of quantum mechanical particles in general, and of the electron in particular.

From the point of view of mathematical formalism, several distinctions arise: One is that the physical problem of the electron in a hydrogen atom is a three-dimensional problem, where only the kinetic part of the quantum mechanical wave equation resembles vibrational wave mechanics. The potential, an important and often troublesome part of the Schrödinger equation, is not involved in the vibrational wave equation. For the hydrogen atom, the attractive interaction between the electron and nucleus confines the electron within the atom, leading to quantization. The separable solutions of the Schrödinger equation are stationary states, with angular and radial nodes arising from imposing radial and angular boundary conditions on the different components of the wave function [32].

A second point that should be made clear is that the shapes obtained are nodes of a wavefunction (vibrational or electronic), not contour plots of the atomic orbital itself. For circular symmetry, the shapes are similar to contour plots (non-zero value cut-outs) of the three-dimensional wavefunction, and could be used as such, although that may cause some confusion at the end of the day. For the s-orbitals, both nodes and non-zero contours are spherical (circular in 2D projection), whereas orbitals with angular dependence (p, d, f and g) have spherical radial nodes and planar and conical angular nodes. Simple diagonal Chladni shapes equivalent to the nodes of a $2p_z$ or the $3d_{xy}$ and $3d_{x^2-y^2}$ orbitals are obtainable, as are the (4 planes, 1 sphere) nodes of the $6g_{z^4}$ orbital (see supporting information) [7]. However, diagonal nodes appear sporadically on centrally-driven circular plates, requiring the usage of higher amplitudes.

Learning objectives: After viewing this demonstration, students should be able to:

1. Explain the idea of a standing wave and how it relates to atomic orbitals
2. Understand the wave-like properties of electrons.
3. Understand the nodal and anti-nodal regions (regions of non-zero amplitude) of an atomic orbital and how it affects the three-dimensional shape of an atomic orbital.

Rather than verbally presenting the atomic orbital as the probability of an electron's position, the aim of this demonstration is to help students qualitatively observe the behaviour of two-dimensional waves, and the meaning of nodal structures in two dimensions. However, the demonstration should open with a presentation introducing the idea of a standing wave, preferably with the use of an example such as the aforementioned guitar string, or a telephone wire fixed at two ends. The especially important point to cover is that standing waves demonstrate low-energy nodes at each higher harmonic equal to the overtone number (first overtone yields one node, the second yields two, and so on). These nodes give the guitar string a particular shape when plucked appropriately because of the nodal and anti-nodal regions.

The wave-like properties of an electron, as explained by Schrödinger's wave equation (see Supporting Material), should be connected to these standing waves. Take the opportunity to have the students consider the shape of such a wave in three-dimensions, vis-à-vis the nodal (see Figure 3 for an example of this on the Chladni plates) and anti-nodal behaviour of a standing wave. This abstract concept is likely to have some students perplexed at which point the Chladni plates demonstration, in which they will observe a two-dimensional example of a standing wave representative of an atomic orbital, ought to be exhibited.

The accessible atomic orbital representations available to the round plate are the 2s, 3s, 4s and 5s orbitals (all but the 4s shown in Figure 3), and the planar nodes of the $3d_{xy}$ orbital can be generated on the square plate (Figure 3d). Table S2 and S3 list the required frequency and amplitude required to generate the desired figures, as well as additional Chladni figure photographs and experimental settings.

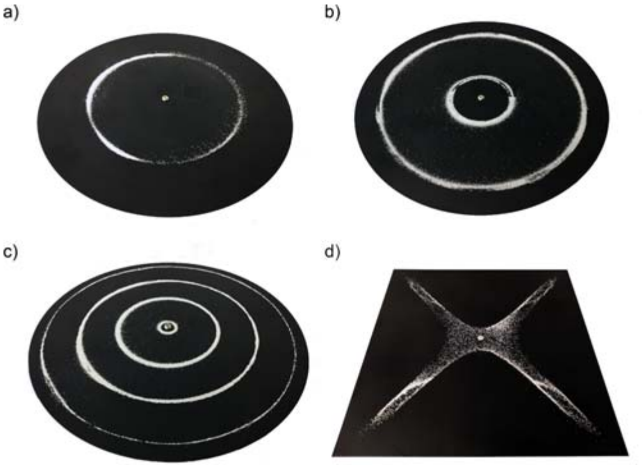

Figure 3. Exemplary standing waves produced on Chladni plates. a) 109 Hz, 300 mVpp (2s orbital), b) 354 Hz, 200 mVpp (3s), c) 1690 Hz, 100 mVpp (5s), d) 84 Hz, 100 mVpp (3d$_{xy}$).

The two-dimensional example may then be explored by producing the node of the 2s orbital (or the 2p orbital) upon the circular Chladni plate. By slowly adjusting the frequency to the harmonic using the frequency generator, an illustration of the standing wave is obtained in real time, as the baking powder is tossed around. Ask students to point out how many nodes are present and relate this to which s orbital is currently being viewed as higher order s orbitals are accessed and to imagine the three-dimensional structure of each Chladni figure.

Post-demonstration Discussion The concept of nodal and anti-nodal regions may then be elaborated on using the figure presently generated on the plate as a reference. Explain that this two-dimensional example illustrates the nodes of an atomic orbital. Following the demonstration, students may be introduced to increasingly complex ideas involving atomic orbitals. Using the 2s Chladni figure as an example, ask the students to point out the most likely position of an electron in a hydrogen atom. Is it inside the circular white line, outside the line, or on the line? Discuss the implications of wave-particle duality of an electron and how this relates to the shape of an atomic orbital, that is, the shape of an atomic orbital is actually a containing surface around a cloud of electron density.

Conclusion

The aim of this demonstration is to help professors introduce atomic orbitals to students. The typical matter of course is to present standing waves and subsequently the properties of atomic orbitals. This is conceivably tricky for students to fully understand due to the nebulous idea of an atomic orbital. It is expected that this exciting demonstration will pique the interest of any student and help them visualize the structure of atomic orbitals as well as fully participate in the discussion which follows.

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Supporting Material. Additional information concerning materials, equipment, and experimental settings, as well as several photos and a video of standing wave patterns generated on the square and circular Chladni plates, may be found within the supporting material.

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