Quantum Analogs

"Acoustic Experiments Modeling Quantum Phenomena"

QA1-A

STUDENT MANUAL

Professor Rene Matzdorf
Universitaet Kassel

A PRODUCT OF TEACHSPIN, INC.

Designed in collaboration with Professor Dr. Rene Matzdorf

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Introduction to TeachSpin's Quantum Analogs

"Quantum Analogs" is TeachSpin's contribution to the teaching of wave mechanics. The idea at the heart of this apparatus is the analogy between the mathematics of the Schrödinger wave equation, and the wave equations that describe the behavior of ordinary sound waves in air. Parts of our acoustic apparatus will allow you to explore acoustic analogs to quantum-mechanical systems in one, and three, dimensions. One of the advantages of the 'acoustic analog' is that sound phenomena occur on a very human scale of length and time.

The hardware you will use is built and supported by TeachSpin, and questions about the hardware should be directed to TeachSpin. All warranty issues will also be handled by TeachSpin.

For several of the investigations in Quantum Analogs you are welcome to use software written and maintained by Prof. Dr. Rene Matzdorf, the developer of the project. This software is free, but comes without any warranty or liability. Be sure to check the internet page Dr. Matzdorf has created, www.physik.uni-kassel.de/quantum-analogs, for program download, manual of the program, frequently asked questions and software updates. The page also offers several excellent visualization programs that you are welcome to download. In case of problems with installation of the connection to the computer you may contact Prof. Matzdorf directly. Bugs in the software may also be reported to be corrected in the next update (matzdorf@physik.uni-kassel.de).

A detailed description of the function of each part of the Controller Box is provided in Appendix 1. Please read it before beginning any experiments.

Quantum Analogs
Chapter 1
Student Manual

Standing Sound Waves in a Tube

An Analog to a Quantum Mechanical Particle in a Box

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1. Standing sound waves in a tube – an analog to a quantum mechanical particle in a box

Objective: For a simple tube, use an oscilloscope to compare the sound input by a speaker at one end to the sound received by a microphone at the other end.

Equipment Required:

TeachSpin Quantum Analog System: Controller, V-Channel & Aluminum Cylinders
Sine wave generator capable of producing 1-50 kHz with a peak-to-peak voltage of 0.50 V
Two-Channel Oscilloscope

Setup:

Make a tube using the tube-pieces. Put the end-piece with the speaker on one end and the end-piece with the microphone on the other. Attach a BNC splitter to *SINE WAVE INPUT* on the Controller. Connect the output of your sine wave generator to one side of the splitter. Use a BNC cable to send the sound signal to the Channel 1 input of your oscilloscope. Plug the lead from the speaker end of your experimental tube to *SPEAKER OUTPUT* on the controller. The same sine wave now goes to both the speaker and Channel 1. Connect the microphone output of the tube array to *MICROPHONE INPUT*. Connect *AC MONITOR* on the Controller to Channel 2 of the oscilloscope. Channel 2 will display the sound signal received by the microphone. Trigger the oscilloscope on Channel 1. Use the *ATTENUATOR* dial on the Controller to keep the signal on Channel 2 from going off scale. (Appendix 1 describes the function of each part of the Controller.)

Experiment:

Start at low frequency (100 Hz or less), and slowly increase the frequency.

Question:

What are you observing? How can you tell that you are at a resonance? Did you notice the phase-shift when going through a resonance? (Note that, due to unknown phase shifts in the speaker, microphone, and electronics, the absolute phase between input and output channel can not be interpreted.)

Experiment:

Change the length of the tube and repeat the experiment.

Question:

Do the resonance frequencies change? Are they higher/lower when the tube is longer/shorter?

Take a full set of data for one tube length:

Measure and record the length of the tube. Measure the first 20 resonance frequencies. Assign the lowest resonance frequency the index number $n = 1$, and plot the resonance frequency f_n as function of its index number, n.

Background:

A resonance occurs when a standing sound wave has developed in the tube. The sound emitted by the speaker is reflected back and forth between the two hard end-walls of the tube. The resonance develops when, after a round trip in the tube, the sound wave is in phase with the wave emitted by the speaker. In this case, the emitted sound interferes with the reflected sound constructively. The condition for resonance is fulfilled when:

$$2L = n\frac{c}{f} = n\lambda$$

with the length of the tube L, the speed of sound c, the frequency f, the wavelength λ and an integer number n=1,2,...∞. Resonances are observed when the tube length is an integer multiple of $\lambda/2$.

Analyze the data:

From the resonance frequencies plotted as function of their index *n,* you can calculate the speed of sound *c*. Make a linear fit for your data. Calculate *c* from the slope and determine the uncertainty of your measurement.

Differential equation for sound and boundary conditions:

The propagation of sound waves in air can be described by differential equations.

On one hand, there is the linearized Euler's equation

$$\frac{\partial \vec{u}}{\partial t} = -\frac{1}{\rho}\,\text{grad}\ p \qquad (1.1)$$

with the velocity of the air $\vec{u}$, the mass density of the air ρ and the pressure p. On the other hand, the continuity equation has to be fulfilled.

$$\frac{\partial \rho}{\partial t} = -\rho\ \mathbf{div}\,\vec{u} \qquad (1.2)$$

Additionally, representing compressibility as κ, the density and the pressure of the air are connected by

$$\frac{\partial p}{\partial \rho} = \frac{1}{\kappa\rho} \qquad (1.3)$$

These equations can be combined to a wave equation for the pressure

$$\frac{\partial^2 p}{\partial t^2} = \frac{1}{\rho\kappa}\Delta p \qquad (1.4)$$

with the Laplace operator Δ. In this wave equation, however, the phase relation between velocity and pressure of the wave is lost, since the velocity has been eliminated. We need to refer to the velocity again, since the boundary conditions at the hard wall can be formulated best with the velocity. It is obvious that, at the surface of the wall, the velocity perpendicular to the wall has to be zero. (The air can not move into or out of the wall.) From eqn. (1.1), it also follows that, at the surface of the wall, the derivative of the pressure in the direction perpendicular to the wall is zero. This combination of boundary conditions is called a "Neumann boundary condition".

For frequencies lower than about 16 kHz, the air is not moving perpendicular to the symmetry-axis (x-axis) of the tube. Thus, $u_y(\vec{r}) = 0$, $u_z(\vec{r}) = 0$, $u_x(\vec{r}) = u_x(x)$ and $p(\vec{r}) = p(x)$.

The problem has now been reduced to a quasi one-dimensional problem and we can make a one-dimensional ansatz for the solution in the form:

$$p(x) = p_0 \cos(kx - \omega t + \alpha) \tag{1.5}$$

Here, p_0 represents the amplitude of the wave and must not be confused with the background air pressure of about 1000 mbar. $\omega = 2\pi f$ is the angular frequency and $k = 2\pi/\lambda$ is the wave vector. This function describes a wave propagating in the positive x-direction. In the tube we find a superposition of right and left (positive and negative x-direction) propagating waves, since the waves are reflected at the ends of the tube. The wavefunction is therefore given by

$$p(x) = \tfrac{1}{2} p_0 \cos(kx - \omega t + \alpha) + \tfrac{1}{2} p_0 \cos(-kx - \omega t - \alpha) \tag{1.6}$$

This can be rewritten as

$$p(x) = p_0 \cos(kx + \alpha)\cos(\omega t) \tag{1.7}$$

Solutions of the differential equation are those wave functions $p(x)$ that fulfill the boundary conditions for a certain tube length L at all times. From the boundary conditions $\mathrm{d}p/\mathrm{d}x(0) = 0$ and $\mathrm{d}p/\mathrm{d}x(L) = 0$, we can easily derive the parameters to be $\alpha = 0$ and $k = n\,\pi/L$.

Dispersion of sound waves:
Redraw your graph of frequency as function of resonance-index (f_n *vs.* n) to show angular frequency as function of wave vector $\omega(k)$. This new graph shows the dispersion relation of sound waves.

Analogy to a quantum mechanical particle in a box:

The sound wave in the tube can serve as an analog for a quantum mechanical particle in a one-dimensional square potential well. The differential equation that describes the particle is Schrödinger's equation:

$$i\hbar \frac{\partial}{\partial t}\psi(\vec{r},t) = -\frac{\hbar^2}{2m}\Delta\psi(\vec{r},t) + V(\vec{r})\psi(\vec{r},t) \tag{1.8}$$

with the wave function $\psi(\vec{r},t)$, the particle mass *m,* and a scalar potential $V(r)$. In the case of a one-dimensional square potential well with infinitely high potential barriers at both ends, and $V = 0$ in the space between the ends, the equation reduces to

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\Delta\psi(x,t) \tag{1.9}$$

This differential equation has as a solution complex waves that are scattered back and forth between the ends of the well. The probability of finding the particle at a certain position x in the well is given by the probability density $|\psi(x,t)|^2$. When multiplied by the elementary charge e, it represents the charge density inside the well.

Most of the solutions of eqn. (1.9) result in time-dependent charge densities. These, however, would emit electromagnetic waves, since charge is moving. On the other hand, there are certain solutions that have a time independent charge density. They can be found by solving the time-independent Schrödinger equation

$$E\psi(\vec{r}) = -\frac{\hbar^2}{2m}\Delta\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) \qquad (1.10)$$

In our case, for the one-dimensional square potential well, the equation simplifies to

$$E\psi(x) = -\frac{\hbar^2}{2m}\Delta\psi(x) \qquad (1.11)$$

This equation can be solved for certain eigenvalues of energy E. We make an ansatz with standing waves of the form

$$\psi(x) = A\sin(kx+\alpha) \qquad (1.12)$$

At the ends of the box, where the potential is infinitely high, the wave function has to be zero (Dirichlet boundary condition). These boundary conditions, $\psi(0) = 0$ and $\psi(L) = 0$, are fulfilled if $\alpha = 0$ and $k = n\ \pi/L$ where n is an integer. The total probability of finding the particle anywhere in the box has to be one. This determines that the amplitude of the wave function is $A = \sqrt{2/L}$.

The solution of Schrödinger's time-dependent equation (1.9) is obtained from the solution (1.12) by multiplying it with a time dependent phase factor

$$\psi(x,t) = A\sin(kx+\alpha)\, e^{-i\omega t} \qquad (1.13)$$

You can convince yourself that, for this solution, $|\psi(x,t)|^2$ is indeed time-independent. The angular frequency in this expression is given by $\omega = E/\hbar$. Note that in quantum mechanics the energy is in general connected with the frequency by

$$E = h\,f = \hbar\omega \qquad (1.14)$$

We can now calculate the eigenvalues of energy that are given by

$$E(k) = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2m\,L^2} \qquad (1.15)$$

This is the dispersion relation of the quantum mechanical particle in a box.

What is analogous, what is different?

The classical sound wave in a tube and the quantum mechanical electron in a square potential well are similar in many respects, but some details are different. Both the sound wave and the wave-function of the electron are solutions of a wave equation describing a delocalized object. The particular aspect being described, however, is different. In the classical case, $p(x,t)$ is the amplitude of the signal picked up by a microphone located at this position. In the quantum mechanical case, the squared amplitude $|\psi(x,t)|^2$ at a certain position gives the probability of finding the electron at this position.

Both of the differential equations have the Laplace operator on the right side (second derivatives with respect to space). However, with respect to time they are different. In the classical case, we have a second derivative with respect to time that leads to wave-solutions. In the quantum mechanical case, the combination of the complex number i and a first-order derivative with respect to time leads to wave solutions. But these wave-solutions are complex due to this special form. It is also the first-order time-derivative that results in a parabolic dispersion $E(k)$ of the electron. In contrast, the sound wave has a linear dispersion due to the second-order time-derivative. Schrödinger's equation includes, in addition, a potential $V(\vec{r})$ that can not be simulated by the sound wave experiment. However, the reflection at a hard wall can be used to function as an analog to an infinitely high potential barrier. In later experiments, we will use irises as an analog for finite potential barriers with certain reflection and transmission probability.

In both cases, eigenstates are found in a well. For certain wavelengths, standing waves are found, and in both cases the wavevector of these waves is given by $k = n\ \pi/L$. However, the position of the nodes is different, because the boundary conditions are not the same. In the quantum mechanical case, the wave function must be zero at the boundary. In the case of sound waves, we have physical quantities that we use to describe the wave. One is the pressure and the other is the air-velocity. Like the quantum mechanical wave function, the velocity has a node at the boundary, but the velocity is a vector. The pressure has a local maximum at the boundary and is a scalar quantity. As an analog to the *scalar* quantum mechanical wave function, we therefore prefer the *scalar* pressure, even though it has an opposite boundary condition. A scalar "velocity potential" could also be used to describe the wave, but it does not help much, since its nodes are at the same position as those for the pressure. You should be aware of this difference.

To each eigenstate, an eigenfrequency, ω, is assigned. In quantum mechanics, it is found in the time dependent phase factor, $e^{i\omega t}$. In the case of sound waves, the eigenfrequency is simply the frequency of the sound itself, $\omega = 2\pi f$. In quantum mechanics, the frequency is directly related to an energy by the equation $E = \hbar\omega$. This has no direct analog in the sound experiments. When working with sound, we look at the frequency of the sound and not at an energy. We therefore consider energy-levels in quantum mechanics as being analogous to the "frequency-levels" in the sound experiments that are given by the sharp resonance frequencies. The dispersion $E(k)$, discussed in quantum mechanics, can be compared with $\omega(k)$ in classical mechanics.

Another little difference is related to the absolute phase. The microphone can measure the phase of the sound wave, but in quantum mechanics the absolute phase of a state can not be measured. Relative phases between two wavefunctions can be measured in quantum mechanics and we can measure the phase of an acoustic wave function at different locations and determine the relative phase to compare with a quantum mechanical system. You should be aware that the sound experiments provide an experimentalist with more information about the system than can be extracted from an analogous quantum mechanical system.

1.2 Measure a spectrum in the tube using an oscilloscope

Objective: In this experiment, the independent variable is the frequency provided by the generator, and the dependent variable is the amplitude of the sound wave reaching the microphone. First, we will examine the amplitude of the sound-wave received at the microphone as a function of the frequency of the sound. Then, we will determine how the spectrum (the pattern) observed depends on the length of the tube conducting the sound.

Setup:

With the tube, speaker and microphone arranged as before, connect the output of the sine wave generator to *SINE WAVE INPUT* on the controller and the wire from the speaker to *SPEAKER OUPUT*. Connect the microphone on the experimental tube to *MICROPHONE INPUT*.

Locate the *FREQUENCY-TO-VOLTAGE CONVERTER* module on the controller and set the toggle switch to *ON*. With the oscilloscope in the xy-mode, connect the *DC-OUTPUT* of the converter module to Channel 1, the x-axis. The converter provides a voltage proportional to the instantaneous frequency. The calibration is 1 V per 1 kHz and it can be used for frequencies up to 10 kHz (or, with offsets, up to 20 kHz).

Connect *DETECTOR OUTPUT* to Channel 2, the y-axis of the oscilloscope. The *DETECTOR OUTPUT* connection provides a dc signal that is proportional to the amplitude of the sound wave at the microphone.

You have now set up the oscilloscope to plot the amplitude of the sound at the microphone as a function of the frequency of the sound.

Set the image persistence time on the oscilloscope to infinite.

Now, sweep the frequency by hand. As you change the frequency, the oscilloscope will plot a spectrum with peaks.

You can use the *DC-OFFSET* knob to center the image on the oscilloscope screen.

Experiment:

Take spectra for different tube lengths and compare them with the results you found in section one.

1.3 Measure a spectrum with the computer and compare it to the spectrum found with the oscilloscope.

Objective: This experiment uses a computer sound card both to generate the sound wave and to sweep its frequency. We will use the oscilloscope to observe the actual sine wave signals both going into the speaker and coming from the microphone. Simultaneously, we will use the computer to display a spectrum which shows the amplitude of the signal from the microphone as a function of the frequency of the sound.

Equipment Required:

TeachSpin Quantum Analog System: Controller, V-Channel & Aluminum Cylinders
Two-Channel Oscilloscope
Two adapter cables (BNC - 3.5 mm plug)
Computer with sound card installed and Quantum Analogs "SpectrumSLC.exe" running

WARNING: The BNC-to-3.5-mm adapter cables are provided as a convenient way to couple signals between the controller and sound card. Unfortunately, they could also provide a way for excessive external voltage sources to damage a sound card. Most sound cards are somewhat protected against excessive inputs, but ***it is the user's responsibility to ensure that adapter cable voltages are kept BELOW 5 Volts peak-to-peak***.
The maximum peak-to-peak value for optimum performance of the Quantum Analogs system depends on your sound card and can vary from 500 mV to 2 V.

Setup:

Using the tube-pieces, make a tube with the end-piece containing the speaker on one end and the end-piece with the microphone on the other.

Now, using connectors on the controller, you will send the sound card signal to both the speaker and Channel 1 of the oscilloscope, and the microphone signal to both the microphone input of the computer and to Channel 2 of the oscilloscope.

First, make sure that the *ATTENUATOR* knob on the controller is set at 0.2 (out of 10) turns.

Let's start with the sound signal. Attach a BNC splitter to *SINE WAVE INPUT* on the controller. Using the adapter cable, connect the output of the sound card to one arm of the splitter. With a BNC cable, convey the sound card signal from the splitter to Channel 1 of your oscilloscope. Plug the lead from the speaker end of your experimental tube to *SPEAKER OUTPUT* on the controller. The sound card signal is now going to both the speaker and Channel 1.

The microphone signal will also be sent two different places. Connect the microphone on your experimental tube to *MICROPHONE INPUT* on the controller. Put a BNC splitter on the controller connector labeled *AC-MONITOR*. From the splitter, use an adapter cable to send the microphone signal to the microphone input on the computer sound card. Use a BNC cable to send the same signal to Channel 2 of the oscilloscope to show the actual signal coming from the microphone.

The computer will plot the instantaneous frequency generated by the sound card on the x-axis and the amplitude of the microphone input signal on the y-axis.

The next job is to start the computer program and adjust the magnitude of both the speaker and microphone signals so that you will have maximum signal while keeping the microphone input to the computer from saturating. Peak-to-peak signals to the microphone input can range from 0.50 to 2.0 volts depending upon your sound card.

Once the program, SpectrumSLC.exe., is running, you can configure the computer. Go to the menu at the top of the screen and choose Configure > Input Channel/Volume At this point, choose *Line In*, if it is available; otherwise choose *Microphone*. On this screen, set the microphone volume slider to the middle of its range.

To set the speaker volume, use the *Amplitude Output Signal* on the lower left of the computer screen. That slider should also be set to middle range.

The microphone signal coming from the apparatus first passes through a built-in amplifier, and then through the *ATTENUATOR,* before reaching the *AC-MONITOR* connector. The ten-turn knob on the attenuator multiplies the incoming signal by a factor ranging from zero to one. For example, a setting of 1.2 turns (out of the 10 turns possible) stands for a transmission of 1.2/10 = 0.12 (or 12%) relative to the maximum possible.

After taking an initial wide range spectrum, choose a section that includes the highest peak and a smaller one next to it. Readjust the scan to cover just this portion. Using the option that allows you to keep successive spectra visible, take Spectrum 1, 2, 3, etc. with the attenuator knob set at 0.1, 0.2, 0.3 . . . turns (out of ten). The changes in the heights of the peaks will tell you whether or not the system is behaving in a linear fashion. Continue to go higher on the 10-turn dial setting until you have visual evidence of saturation.

Once you have reached saturation, drop back into the linear range. Now you can operate with confidence that the signals you see really are proportional to the amplitude of the sound wave you are studying.

Experiment:

Now you can use the computer to collect an overview spectrum from about 100 to 10,000 Hz. You can use coarse steps (~10 Hz) and a short time per step (~50 ms) for this investigation. As the frequency is changing, watch the trace on the oscilloscope. How is the oscilloscope showing the change in frequency? What is happening to the amplitude of the signal? How is this related to the trace being created on the computer?

Compare the spectrum recorded on the computer to the results you found using the oscilloscope in the first experiment.

Linewidth:

Lifetime of quantum mechanical states

In most cases eigenstates do not last forever. In classical physics there is decay due to dissipation of energy by friction. In quantum mechanics only the ground state lasts forever. Excited states with higher energy decay into the ground state, which is the eigenstate of the system with the lowest energy. These effects are not included in the differential equations. However, we can introduce the decay easily into the wave functions by replacing the time dependent factors in the wave function $\cos(\omega t)$ and $e^{i\omega t}$, respectively, with a factor that is oscillating and exponentially damped. With a damping constant λ it results in $e^{-\lambda t}\cos(\omega t)$ and $e^{-\lambda t - i\omega t}$, respectively.

In the case of finite lifetime, the wave function cannot be assigned to a single angular frequency ω_0 but contains a spectrum of angular frequencies that we can determine by Fourier-transformation. Let's write the wave function in a general way as

$$\psi(x,t) = f(x)\, e^{-(\lambda + i\omega_0)t} \qquad (1.16)$$

with an arbitrary spatial dependence $f(x)$. For t < 0, the wave function is assumed to be zero. By performing a Fourier-transformation we obtain the so-called spectral function, $A(\omega)$, that describes the amplitude as function of angular frequency in the classical case. In the quantum mechanical case, $|A(\omega)|^2$ is the probability of measuring the particle to have the energy $E = \hbar\omega$. Performing the Fourier-transformation

$$A(\omega) = \frac{1}{\sqrt{2\pi}} \int_0^\infty e^{-(\lambda + i\omega_0)t}\, e^{i\omega t}\, \mathrm{d}t \qquad (1.17)$$

we obtain the spectral function

$$A(\omega) = \frac{\frac{1}{\sqrt{2\pi}}}{\lambda + i(\omega_0 - \omega)} \;. \qquad (1.18)$$

The absolute squared is a so-called Lorentzian peak

$$|A(\omega)|^2 = \frac{\frac{1}{2\pi}}{(\omega_0 - \omega)^2 + \lambda^2} \,. \qquad (1.19)$$

The width of the peak is directly related to the lifetime τ of the eigenstate. The lifetime denotes the time after that the amplitude of the state has been reduced to 1/e. From the half width at half maximum of the peak the damping constant λ can be read directly. In quantum mechanics the width in energy Γ of a metastable state is $\Gamma = \hbar\lambda$

$$\Gamma = \frac{\hbar}{\tau} \qquad (1.20)$$

The spectral function $A(\omega)$ is complex, which can be written as the absolute $|A(\omega)|$ multiplied by a complex phase factor $A(\omega) = |A(\omega)| e^{i\varphi}$. Both amplitude and phase depend on the angular frequency.

Linewidth of the resonances in the sound experiment

In the sound experiments the situation is a little bit different, but the result looks almost the same as in quantum mechanics. The sound wave close to an eigenstate can be seen as a damped, driven harmonic oscillator described by the linear differential equation

$$\frac{\mathbf{d}^2 p}{\mathbf{d}t^2} + 2\gamma \frac{\mathbf{d}p}{\mathbf{d}t} + \omega_0^2 p = K\cos(\omega t) \tag{1.21}$$

This driving force is represented by the speaker that is driving the standing sound wave. The resonance frequency under consideration has the angular frequency ω_0. The solution of this differential equation is a superposition of a transient solution that is a solution of the homogenous differential equation (first part of eqn. 1.22), and a steady-state solution (second part of eqn. 1.22) that is of interest here.

$$p(t) = A_1 e^{-\gamma t}\cos(\omega_1 t + \varphi_1) + A\cos(\omega t + \varphi) \tag{1.22}$$

For our experiment, we can assume that the transient solution has already damped out, so that we are detecting only the steady state amplitude, A, of the sound wave. This amplitude depends on the frequency ω of the driving force compared to the eigen-frequency ω_0 of the oscillator. It is given by

$$A = \frac{K}{\sqrt{(\omega_0^2 - \omega^2)^2 + (2\gamma\omega)^2}} \quad . \tag{1.23}$$

The phase between driving force and oscillating air is given by

$$\varphi = \arctan\frac{2\gamma\omega}{\omega_0^2 - \omega^2} \,. \tag{1.24}$$

Using the complex exponential function, the result can be written even more simply.

For this purpose we write the differential equation in the form

$$\frac{\mathbf{d}^2 p}{\mathbf{d}t^2} + 2\gamma \frac{\mathbf{d}p}{\mathbf{d}t} + \omega_0^2 p = Ke^{i\omega t} \tag{1.25}$$

and the steady-state solution as

$$p_s(t) = Ae^{i(\omega t + \varphi)} \,. \tag{1.26}$$

The complex amplitude A as function of angular frequency ω can then be written as

$$A = \frac{Ke^{i\varphi}}{\omega_0^2 - \omega^2 + 2i\gamma\omega} \,. \tag{1.27}$$

If only single resonance existed in the tube, the microphone would measure the amplitude

$$|A| = \left| \frac{K e^{i\varphi}}{\omega_0^2 - \omega^2 + 2i\gamma\omega} \right| = \frac{K}{\sqrt{(\omega_0^2 - \omega^2)^2 + (2\gamma\omega)^2}} . \qquad (1.28)$$

In reality, however, there are a number of resonances, all of which are simultaneously excited. The superposition is coherent because there is a fixed phase-relation between the different resonances.

The entire spectrum is therefore a superposition of all complex amplitudes. That can be written as:

$$|A| = \left| \frac{K_1 e^{i\varphi_1}}{\omega_1^2 - \omega^2 + 2i\gamma_1\omega} + \frac{K_2 e^{i\varphi_2}}{\omega_2^2 - \omega^2 + 2i\gamma_2\omega} + \frac{K_3 e^{i\varphi_3}}{\omega_3^2 - \omega^2 + 2i\gamma_3\omega} + \ldots \right|$$

$$|A(\omega)| = \left| \sum_{i=1}^{n} \frac{K_i e^{i\varphi_i}}{\omega_i^2 - \omega^2 + 2i\gamma_i\omega} \right| \qquad (1.29)$$

In this notation, we are using four fitting parameters to model each peak in the spectrum: K_i, $\omega_i, \gamma_i, \varphi_i$. In our simplified theoretical model we describe the resonances in the tube by independent damped, driven oscillators with parameters taken from the experiment. The coupling of the speaker to the standing wave depends on geometry and can be different for different resonances, which results in different K_i's. The friction depends on a different parameter, which results in different γ_i's. Finally, the phase between driving force and oscillating air is also different for different resonances. Therefore, the phase φ_i is also fitted as a parameter.

In a spectrum measured with an oscilloscope or by computer, $|A(\omega)|$ is plotted. The connector marked *DC-OUTPUT* on the Quantum Analogs controller gives a voltage proportional to $|A(\omega)|$. The linewidth of an acoustic resonance is small compared to its frequency; $\gamma << \omega_0$. In this case we can make the approximation

$$\omega_0 + \omega \approx 2\omega \quad \Rightarrow \quad \omega_0^2 - \omega^2 \approx 2\omega(\omega_0 - \omega)$$

and rewrite the absolute value of Amplitude as

$$A(\omega) \approx \frac{K e^{i\varphi}}{2i\omega\left[\gamma + i(\omega - \omega_0)\right]}$$

Since ω can be assumed to be almost constant in the frequency interval across the peak (within the approximation $\gamma << \omega_0$),

$$A(\omega) \propto \frac{1}{\gamma + i(\omega - \omega_0)}$$

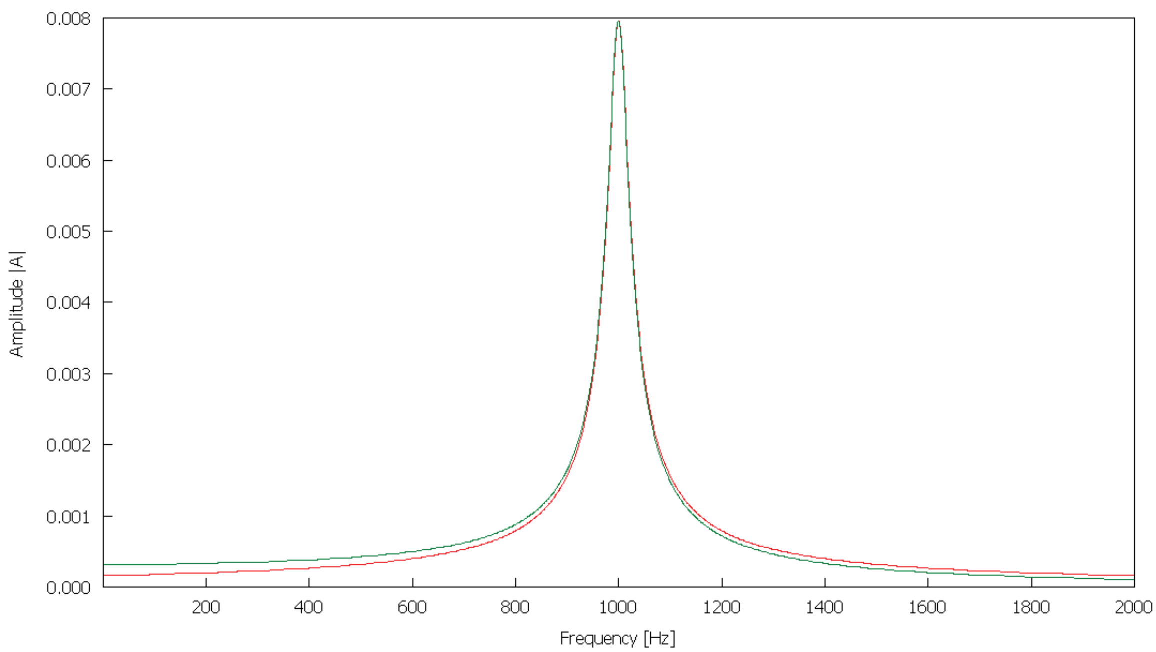
The resonance peak $A(\omega)$, in a classical driven, damped oscillator has the same shape as the spectral function of quantum mechanical eigenstate with finite lifetime (eqn. 1.18).
In the following figure the two line-shapes

$$|A(\omega)| = \frac{2\omega_0}{\sqrt{(\omega_0^2 - \omega^2)^2 + (2\gamma\omega)^2}}$$

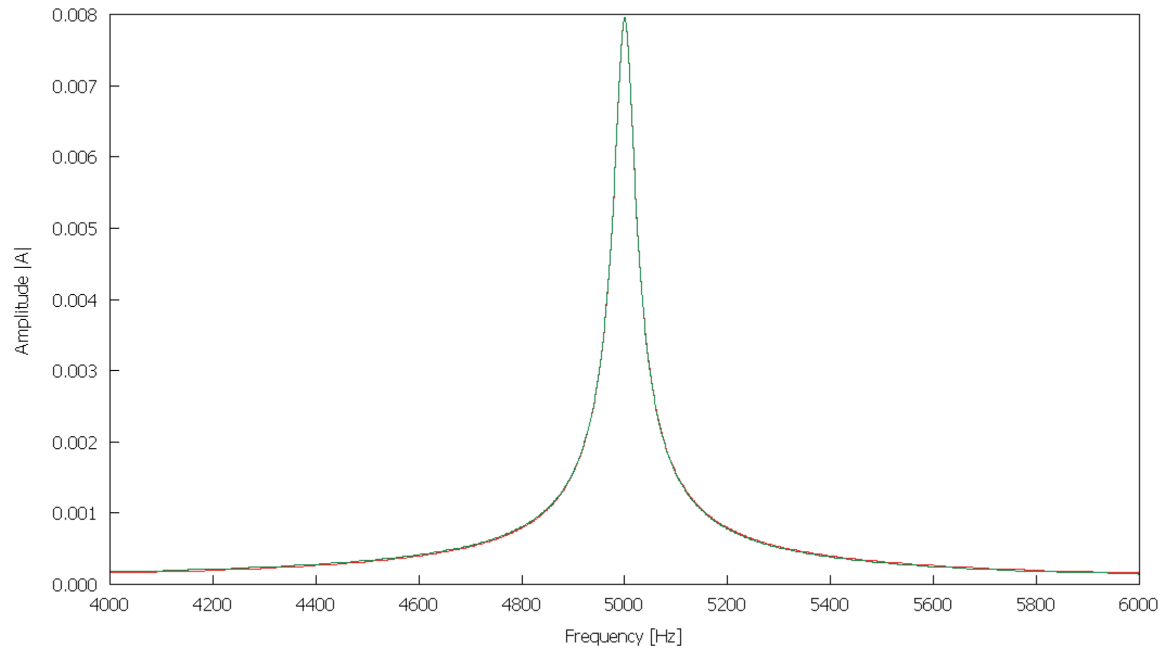
and

$$|A(\omega)| = \frac{1}{\sqrt{(\omega_0 - \omega)^2 + \lambda^2}}$$

are plotted for comparison with the parameter $\omega_0 = 2\pi \cdot 1000\text{Hz}$ and $\gamma = \lambda = 2\pi \cdot 20\text{Hz}$. The full width at half maximum of the peaks is $\Delta\omega = 2\sqrt{3}\lambda$ and $\Delta f = \frac{\sqrt{3}}{\pi}\lambda$, respectively.

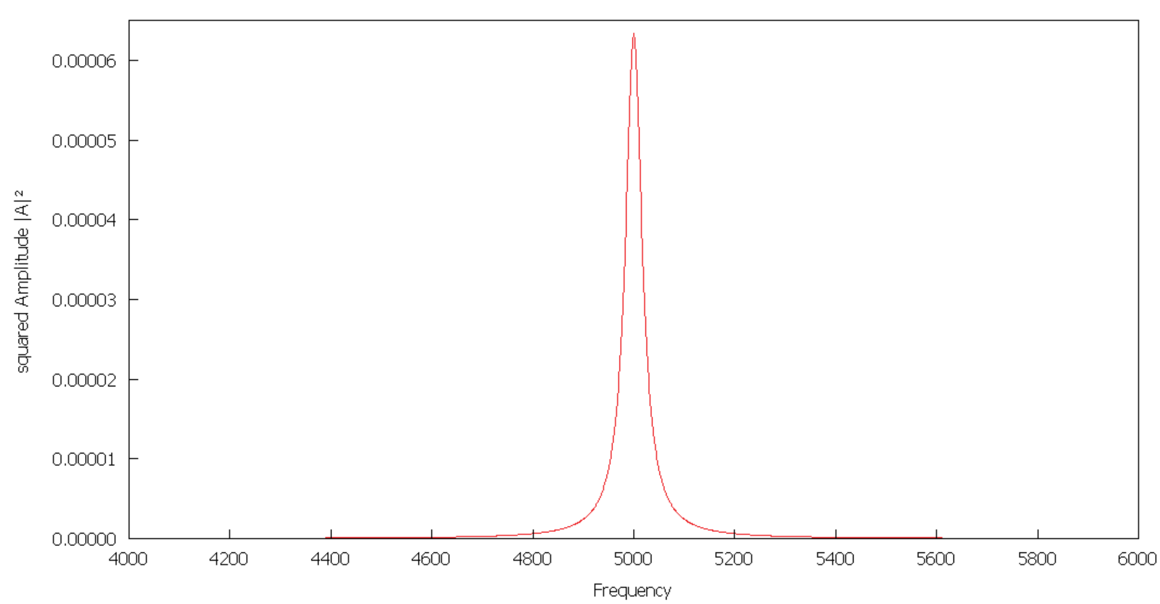


Line-shape of a classical resonance (green line) and for a quantum mechanical eigenstate with finite lifetime (red line) for comparison (parameter see text).



A comparison of the line-shape of a classical resonance (green line) and a quantum mechanical eigenstate with finite lifetime (red line).
Parameters: $\omega_0 = 2\pi \cdot 5000\text{Hz}$ and $\gamma = \lambda = 2\pi \cdot 20\text{Hz}$.

The better known Lorentzian-shape for the same parameter looks as follows



Lorentzian line-shape (squared amplitude) of a quantum mechanical eigenstate with finite lifetime
Parameters: $\omega_0 = 2\pi \cdot 5000\text{Hz}$ and $\gamma = \lambda = 2\pi \cdot 20\text{Hz}$

Objective: In this experiment, we will use the computer to record a spectrum of eight or fewer peaks. We will then use the software program provided to demonstrate that the data generated by Quantum Analogs can be fit to the theoretical models.

Setup:

Create a short tube and set the computer parameters to produce a spectrum with eight or fewer peaks. One possible configuration would be a 150 mm long tube, a sweep from 5000 Hz to 14000 Hz, 5 Hz steps, and 50 ms per step.

Experiment:

Generate a spectrum of eight or fewer peaks. After generating your spectrum, open the fitting window in the software via the sequence: Menu > Windows > Fit. In the fitting window that opens, your first task is to give the software a set of initial estimates for the location and height of up to eight resonances. In the 'Peak Number' menu at the upper left of the window, select Peak 1. Now, point your mouse to the top of the lowest frequency peak, and left-click your mouse. You will see (in blue) the theoretical resonance with the center and height matching the peak you have selected. The blue curve also has a default value for width. If you have a mouse wheel, you may use the wheel to adjust the width estimate to match your data. Perfection is not required in these initial estimates.

When you are done with Peak 1, right-click your mouse and the selection in the Peak Number menu will change to Peak 2. Now locate and left-click the second peak. Repeat this initial-estimate procedure for it and each subsequent peak.

After using the mouse to put in the initial estimates for all of the peaks, you will see a blue curve showing a first approximation of the theoretical model. Now click the button for 'Start Fit', and the software will use your estimates to optimize the match between the data curve (red) and the theoretical model (blue), by adjusting the fitting parameters. If one of the model's peaks 'escapes' from the data of the spectrum during this fitting procedure, you can stop the fit and readjust manually. After you've reset that peak's estimated parameters, just restart the automatic fit.

When the automatic fitting is done, you can use the Peak Number menu (at the window's upper left) to select any peak. The software then shows the values of the parameters for that peak that best-fit your data.

You can now check the repeatability of your data. To do this, first record the parameters for one of your peaks. Next, acquire a fresh set of data. Repeat the fitting procedure, and look again for the center location of your chosen peak. (Prepare to be very impressed!)

You can save the fitting parameters that you generated as an ASCII file. The best-fit theoretical function can be saved either as a data file or an image file.

Quantum Analogs
Chapter 2

Student Manual

Modeling a Hydrogen Atom
with a
Spherical Resonator

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Universitaet Kassel

2. Modeling a hydrogen atom with a spherical resonator

Background:

The hydrogen atom, with a single electron in the Coulomb potential of the nucleus, is an ideal object for studying the basic principles of atomic physics. As the simplest of all atoms, without any electron correlations, it can be solved analytically.

The spherical symmetry of the three-dimensional problem makes it possible to separate the angular and radial variables for the solution of Schrödinger's equation. The acoustic analog uses a spherical resonator that allows a separation of variables for the solution of the Helmholtz equation in the same way as is done for the hydrogen atom. We will see that the eigenfunctions with respect to the angular variables – the spherical harmonics $Y_l^m(\theta,\varphi)$ – are exactly the same for both problems. The radial eigenfunctions, however, are different.

The three-dimensional Schrödinger equation

$$E\psi(\vec{r}) = -\frac{\hbar^2}{2m}\Delta\psi(\vec{r}) - \frac{e^2}{r}\psi(\vec{r}) \tag{2.1}$$

expressed in polar coordinates

$$E\psi = \frac{\hbar^2}{2mr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{\hbar^2}{2mr^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{\hbar^2}{2mr^2\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2} - \frac{e^2}{r}\psi$$

can be separated in two differential equations with the ansatz

$$\psi(r,\theta,\varphi) = Y_l^m(\theta,\varphi)\ \chi_l(r). \tag{2.2}$$

The spherical harmonics are solutions of the differential equation

$$-\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]Y_l^m(\theta,\varphi) = l(l+1)\,Y_l^m(\theta,\varphi) \tag{2.3}$$

and $\chi_l(r)$ is a solution of the so called radial equation

$$-\frac{\hbar^2}{2mr}\frac{\partial^2}{\partial r^2}r\chi(r) - \frac{l(l+1)\hbar^2}{2mr^2}\chi(r) - \frac{e^2}{r}\chi(r) = E\chi(r). \tag{2.4}$$

In the case of the spherical acoustic resonator we transform eqn. 1.4

$$\frac{\partial^2 p}{\partial t^2} = \frac{1}{\rho\kappa}\Delta p \tag{2.5}$$

with the ansatz $p(\vec{r},t) = p(\vec{r})\cos(\omega t)$ into the time independent Helmholtz equation

$$\omega^2 p(\vec{r}) = -\frac{1}{\rho\kappa}\Delta p(\vec{r}), \tag{2.6}$$

Using c as the speed of sound, equation 2.6 can be written as

$$-\frac{\omega^2}{c^2}p(\vec{r}) = \Delta p(\vec{r}) \tag{2.7}$$

The Helmholtz equation in polar coordinates is given by

$$-\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial p}{\partial r}\right)-\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial p}{\partial\theta}\right)-\frac{1}{r^2\sin^2\theta}\frac{\partial^2 p}{\partial\varphi^2}=\frac{\omega^2}{c^2}p$$

It separates into a radial-function *f(r)* and the spherical harmonics $Y_l^m(\theta,\varphi)$.

$$p(r,\theta,\varphi)=Y_l^m(\theta,\varphi)\,f(r) \tag{2.8}$$

With this ansatz the Helmholtz equation is separated in one differential equation for the spherical harmonics

$$-\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]Y_l^m(\theta,\varphi)=l(l+1)\,Y_l^m(\theta,\varphi) \tag{2.9}$$

and another for the radial function

$$-\frac{\partial^2 f}{\partial r^2}-\frac{2}{r}\frac{\partial f}{\partial r}+\frac{l(l+1)}{r^2}f(r)=\frac{\omega^2}{c^2}f(r) \tag{2.10}$$

You see immediately that eqn. 2.3 and eqn. 2.9 are exactly the same and have the same eigenfunctions and eigenvalues for the quantum numbers *l* (angular momentum or azimuthal quantum number) and *m* (magnetic quantum number). The radial equations are different, which, of course, results in different solutions. The Coulomb potential only appears in the radial equation (eqn. 2.4). Therefore, it does not affect the spherical harmonics. The eigenvalues of the radial equations are numerated by the quantum number n' (radial quantum number).

The energy levels $E_{n'l}$ of the hydrogen atom are the eigenvalues of the radial equation (2.4) and the eigenfrequencies of the spherical acoustic resonator $\omega_{n'l}$ are eigenvalues of the radial equation (2.10). Since the two differential equations are of different form, the resonance frequencies in the resonator can not be compared quantitatively with the energy levels of the hydrogen atom. However, the resonances can be classified with the same quantum numbers n' (radial quantum number), *l* (azimuthal quantum number) and *m* (magnetic quantum number). The quantum numbers are integers and

$$n'\geq 0 \qquad l\geq 0 \qquad -l\leq m\leq l \tag{2.11}$$

In the non-relativistic description of the hydrogen atom, many energy levels are degenerate, due to the special form of the Coulomb potential. The energies can be written in the form

$$E_{n'l}=-\left(\frac{e^2}{\hbar c}\right)^2\frac{mc^2}{2(l+1+n')^2}. \tag{2.12}$$

All levels with the same value for $(l+1+n')$ are degenerate. Therefore, a new quantum number is introduced that is called the "principal quantum number" *n*. It is given by

$$n=l+1+n' \tag{2.13}$$

For a given principal quantum number *n* the azimuthal quantum number *l* can take the values

$$0\leq l\leq n-1 \tag{2.14}$$

even though it runs to infinity for a given radial quantum number.

In the diagrams of the hydrogen atom spectrum shown below, the energy levels are labeled in two different ways. In the left figure they are labeled in the ordinary manner, using the principal quantum number. The right figure shows the energy levels labeled using the radial quantum number.

(4,0)=4s (4,1)=4p (4,2)=4d (4,3)=4f

(3,0)=3s (3,1)=3p (3,2)=3d

(2,0)=2s (2,1)=2p

(1,0)=1s

Energy levels of the hydrogen atom labeled with the principal quantum number in the ordinary way (n,l).

(3,0)=4s (2,1)=4p (1,2)=4d (0,3)=4f

(2,0)=3s (1,1)=3p (0,2)=3d

(1,0)=2s (0,1)=2p

(0,0)=1s

Energy levels of the hydrogen atom labeled with the radial quantum number (n',l).

The degeneracy of levels with the same principal quantum number does not have an analog in the spherical acoustic resonator, since the radial equation is different.

In the spherically symmetric case, the eigenvalues for different magnetic quantum numbers *m* are degenerate for any form of the radial equation. This is true for both the hydrogen atom and the spherical acoustic resonator. In general, the eigenvalues numbered by the quantum numbers (n,l) or by (n',l) are $(2l+1)$-fold degenerate. This degeneracy is lifted when the spherical symmetry is broken.

Now let's do some experiments that allow us to see many of these effects. First, we will identify the resonances by their angular dependence.

2.1 Measure resonances in the spherical resonator and determine their quantum numbers

Objective: Determine the resonance frequencies for the spherical resonator and gather data to determine their angular-momentum quantum numbers.

Equipment Required:

TeachSpin Quantum Analog System: Controller, Hemispheres, Accessories
Sine wave generator capable of producing 1-50 kHz with a peak-to-peak voltage of 0.50 V
Two-Channel Oscilloscope

Setup:

Assemble the hemispheres so that the speaker is in the lower hemisphere and the microphone in the upper. Attach a BNC splitter to *SINE WAVE INPUT* on the controller. Connect the output of your sine wave generator to one side of the splitter. Use a BNC cable to send the sound signal to Channel 1 of the oscilloscope. Plug the lead from the speaker on the lower hemisphere to *SPEAKER OUTPUT* on the controller. The same sine wave now goes to both the speaker and Channel 1.

Use a BNC cable to connect the microphone output from the upper hemisphere to *MICROPHONE INPUT*. Connect *AC MONITOR* on the controller to Channel 2 of the oscilloscope to display the sound signal received by the microphone. Trigger the oscilloscope on Channel 1.

Use the *ATTENUATOR* dial on the Controller to keep the signal on Channel 2 from going off scale. (Appendix 1 describes the function of each part of the Controller.)

Adjust the position of the upper hemisphere so that α =180° on the scale is at the reference mark. In this position, the microphone and speaker are at opposite ends of a diameter.

Experiment:

Start at a low frequency and sweep the frequency up to about 8 kHz (8,000 Hz).

Write down all the resonance frequencies you observe. (If you listen carefully, you may actually hear some of them.)

Objective:

Observe, qualitatively, the way the amplitude of the resonance signal depends on the location of the microphone.

Experiment:

We will now gather data that will allow us to infer the angular quantum numbers of the resonances. Go to the second resonance, at about 3680 Hz. Fine-tune the frequency until it is as close as possible to the peak of the resonance. Shift the curves on the oscilloscope horizontally so that a maximum of the microphone signal (Channel 2) is located in the center of the image and marked by a vertical line. Now, watching the signal on the oscilloscope, slowly rotate the upper hemisphere, with respect to the lower one, from $\alpha = 180°$ to $\alpha = 0°$.

Questions:

How did the amplitude change? Did the signal change its sign? Determine the angle where the amplitude is zero. At which angles is the signal maximal? Do both extrema have the same amplitude?

Note: Do not warm the aluminum parts too much by touching them with your hands. The speed of sound is temperature-dependent, and, in consequence, the resonance frequency would shift with temperature. While analyzing the angular dependence, the chosen generator frequency should remain on top of the resonance.

Analyze the data:

The angle α read on the scale is not a suitable angle for comparison with theory. To analyze the data, you must first use α to calculate the polar angle, θ, which we have used for polar coordinates. Both the speaker and microphone are at an angle of 45° with respect to the horizontal plane between the hemispheres. By rotating the hemispheres with respect to each other, the angle θ can be changed from $\theta = 90°$ (at $\alpha = 0°$) to $\theta = 180°$ (at $\alpha = 180°$). Intermediate angles can be calculated using the formula

$$\theta = \arccos(\tfrac{1}{2}\cos\alpha - \tfrac{1}{2})\,. \qquad (2.15)$$

You have measured the θ-dependence of the spherical harmonic function $Y_l^m(\theta,\varphi)$ with $l = 2$ and $m = 0$. Now we need to learn more about the spherical harmonics to compare the experiment with theory.

Spherical Harmonics and Legendre Polynomials:

The spherical harmonics $Y_l^m(\theta,\varphi)$ can be written as

$$Y_l^m(\theta,\varphi) \propto P_l^m(\cos\theta)\, e^{im\varphi} \tag{2.16}$$

in terms of the associated Legendre polynomials P_l^m. For these experiments, we can restrict ourselves to the case m = 0, because our speaker creates waves with cylindrical symmetry about the speaker axis. For m = 0 the spherical harmonics do not have a φ-dependence and the wave function has the same amplitude for all azimuthal angles ,φ. The dependence on the polar angle θ is given by the Legendre polynomials

$$Y_l^0(\theta,\varphi) \propto P_l^0(\cos\theta) \tag{2.17}$$

The first nine Legendre polynomials are shown below:

$$P_0(\cos\theta) = 1$$
$$P_1(\cos\theta) = \cos\theta$$
$$P_2(\cos\theta) = \frac{1}{2}(3\cos^2\theta - 1)$$
$$P_3(\cos\theta) = \frac{1}{2}(5\cos^3\theta - 3\cos\theta)$$
$$P_4(\cos\theta) = \frac{1}{8}(35\cos^4\theta - 30\cos^2\theta + 3)$$
$$P_5(\cos\theta) = \frac{1}{8}(63\cos^5\theta - 70\cos^3\theta + 15\cos\theta)$$
$$P_6(\cos\theta) = \frac{1}{16}(231\cos^6\theta - 315\cos^4\theta + 105\cos^2\theta - 5)$$
$$P_7(\cos\theta) = \frac{1}{16}(429\cos^7\theta - 693\cos^5\theta + 315\cos^3\theta - 35\cos\theta)$$
$$P_8(\cos\theta) = \frac{1}{128}(6435\cos^8\theta - 12012\cos^6\theta + 6930\cos^4\theta - 1260\cos^2\theta + 35)$$

In Fig. 2.1 and 2.2 the first six Legendre polynomials are plotted. The number of nodes in each Legendre polynomial is equal to the azimuthal quantum number *l*.

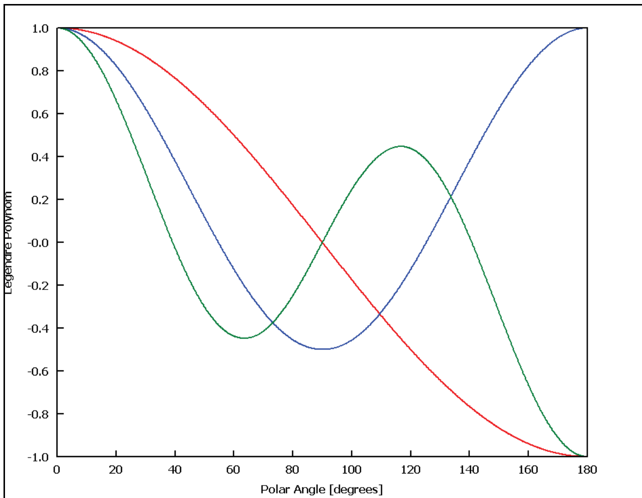


Fig. 2.1: Legendre Polynomials

$P_1(\cos\theta) = \cos\theta$ in red,

$P_2(\cos\theta) = \frac{1}{2}(3\cos^2\theta - 1)$ in blue and

$P_3(\cos\theta) = \frac{1}{2}(5\cos^3\theta - 3\cos\theta)$ in green.

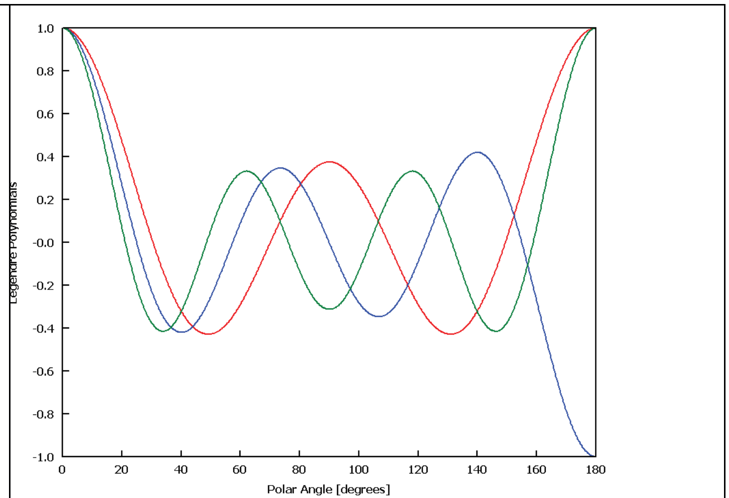


Fig. 2.2: Legendre Polynomials

$P_4(\cos\theta) = \frac{1}{8}(35\cos^4\theta - 30\cos^2\theta + 3)$ in red,

$P_5(\cos\theta) = \frac{1}{8}(63\cos^5\theta - 70\cos^3\theta + 15\cos\theta)$ in blue

$P_6(\cos\theta) = \frac{1}{16}(231\cos^6\theta - 315\cos^4\theta + 105\cos^2\theta - 5)$ in green.

In the following table, the nodes of the Legendre polynomials are listed. **Be aware that these are the polar angles θ, and not the angles you read on the scale.**

P_0								
P_1	90°							
P_2	54.74°	125.26°						
P_3	39.23°	90°	140.77°					
P_4	30.56°	70.12°	109.88°	149.44°				
P_5	25.02°	57.42°	90°	122.58°	154.98°			
P_6	21.18°	48.61°	76.19°	103.81°	131.39°	158.82°		
P_7	18.36°	42.14°	66.06°	90°	113.94°	137.86°	161.64°	
P_8	16.20°	37.19°	58.30°	79.43°	100.57°	121.70°	142.81°	163.80°

Table 2.1: Nodes of the first eight Legendre polynomials, given in the polar angles θ.

Questions:

Now you can identify the angular quantum number l of the second resonance you have measured.

As you varied α from 180° to 0°, what range of θ did you cover?

How many nodes did you discover in the range you covered?

Based on your observations, to what l value does the resonance you examined correspond?

Does the θ angle measurement of the node you have measured agree with the angle predicted by the theory?

Do the relative magnitudes of the extrema fit to the theory?

Note about the magnetic quantum number:

The resonance that you have analyzed is $(2l+1)$-fold degenerate with respect to the magnetic quantum number m. However, in this experiment we observe almost exclusively the $m = 0$ state. The standing sound wave in the sphere is driven by the local speaker. The speaker defines the z-axis of the problem. It emits a wave traveling more or less back and forth along the z-axis and having cylindrical symmetry around that axis. This symmetry of the standing wave is described by the $m = 0$ state. States with other $m \neq 0$ describe waves that move on an orbit inside the sphere. These types of waves are much less effectively driven by our speaker located on the z-axis, since these states have nodes at $\theta = 0°$ and $\theta = 180°$.

Objective: We will trace out the angular dependence of the amplitude of the wave function.

Additional Apparatus: dc voltmeter

Setup:

As in the first part of this experiment, attach a BNC splitter to *SINE WAVE INPUT* on the controller. Connect the output of your sine wave generator to one side of the splitter. Use a BNC cable to send the sound signal to Channel 1 of the oscilloscope. Plug the lead from the speaker on the lower hemisphere to *SPEAKER OUTPUT* on the controller. The same sine wave now goes to both the speaker and Channel 1.

Use a BNC cable to connect the microphone output from the upper hemisphere to *MICROPHONE INPUT*. Connect *AC MONITOR* on the controller to Channel 2 of the oscilloscope to display the sound signal received by the microphone. Trigger the oscilloscope on Channel 1.

This time put the upper hemisphere in the position α = 0° on the scale. In this position the microphone is directly above the speaker which means angle θ will be 90°.

To observe the amplitude of the sound signal at the microphone, connect a voltmeter to *DETECTOR-OUTPUT*. You should also observe the sound signal itself by connecting the *AC-MONITOR* on the controller with Channel 2 of the oscilloscope. Trigger the oscilloscope to Channel 1.

Experiment:

For a couple of major resonances, measure the amplitude as function of the angle α. You can read the absolute value of the amplitude on the voltmeter and use the oscilloscope to determine the sign.

Record the nodes (angle at which the amplitude is zero) for the same resonances.

Analyze the data:

Plot your data as function of the polar angle θ and fit the data with the Legendre polynomial that is the best match. Do this for all the resonances you have measured.

Compare the nodes you have measured with the nodes of the corresponding Legendre polynomial given in table 2.1.

Note:

Some of the resonances are very close to each other so that the peaks are overlapping. This will result in a superposition of two wavefunctions with different quantum numbers. In this case, the angular dependence you have measured does not fit to a single Legendre polynomial. We will analyze these cases in more detail by taking spectra with the computer.

2.2 Measure spectra and wavefunctions in the spherical resonator with the computer

Objective: In this experiment, you will use a computer sound card both to generate the sound wave and to sweep its frequency. You will use the oscilloscope to observe the actual sine wave signals both going into the speaker and coming from the microphone. Simultaneously, you will use the computer to display a spectrum which shows the amplitude of the signal from the microphone as a function of the frequency of the sound.

Equipment Required:

TeachSpin Quantum Analog System: Controller, Hemispheres, Accessories
Two-Channel Oscilloscope
Two adapter cables (BNC - 3.5 mm plug)
Computer with sound card installed and Quantum Analogs "SpectrumSLC.exe" running

WARNING: The BNC-to-3.5-mm adapter cables are provided as a convenient way to couple signals between the controller and sound card. Unfortunately, they could also provide a way for excessive external voltage sources to damage a sound card. Most sound cards are somewhat protected against excessive inputs, but ***it is the user's responsibility to ensure that adapter cable voltages are kept BELOW 5 Volts peak-to-peak***.
The maximum peak-to-peak value for optimum performance of the Quantum Analogs system depends on your sound card and can vary from 500 mV to 2 V.

Setup:

Now, using connectors on the controller, you will send the sound card signal to both the speaker and Channel 1 of the oscilloscope, and the microphone signal to both the microphone input of the computer and to Channel 2 of the oscilloscope.

First, make sure that the *ATTENUATOR* knob on the controller is set at 0.2 (out of 10) turns.

Let's start with the sound signal. Attach a BNC splitter to *SINE WAVE INPUT* on the controller. Using the adapter cable, connect the output of the sound card to one arm of the splitter. With a BNC cable, convey the sound card signal from the splitter to Channel 1 of your oscilloscope. Plug the lead from the speaker on the lower hemisphere to *SPEAKER OUTPUT* on the controller. The sound card signal is now going to both the speaker and Channel 1.

The microphone signal will also be sent two different places. Connect the microphone on the upper hemisphere to *MICROPHONE INPUT* on the controller. Put a BNC splitter on the controller connector labeled *AC-MONITOR*. From the splitter, use an adapter cable to send the microphone signal to the microphone input on the computer sound card. Use a BNC cable to send the same signal to Channel 2 of the oscilloscope to show the actual signal coming from the microphone.

The computer will plot the instantaneous frequency generated by the sound card on the x-axis and the amplitude of the microphone input signal on the y-axis.

The next job is to start the computer program and adjust the magnitude of both the speaker and microphone signals so that you will have maximum signal while keeping the microphone input to the computer from saturating. Peak-to-peak signals to the microphone input can range from 0.50 to 2.0 volts depending upon your sound card.

Once the program, SpectrumSLC.exe., is running, you can configure the computer. Go to the menu at the top of the screen and choose Configure > Input Channel/Volume At this point, choose *Line In*, if it is available; otherwise choose *Microphone*. On this screen, set the microphone volume slider to the middle of its range.

To set the speaker volume, use the *Amplitude Output Signal* on the lower left of the computer screen. That slider should also be set to middle range.

The microphone signal coming from the apparatus first passes through a built-in amplifier, and then through the *ATTENUATOR,* before reaching the *AC-MONITOR* connector. The ten-turn knob on the attenuator multiplies the incoming signal by a factor ranging from zero to one. For example, a setting of 1.2 turns (out of the 10 turns possible) stands for a transmission of 1.2/10 = 0.12 (or 12%) relative to the maximum possible.

After taking an initial wide range spectrum, choose a section that includes the highest peak and a smaller one next to it. Readjust the scan to cover just this portion. Using the option that allows you to keep successive spectra visible, take Spectrum 1, 2, 3, etc. with the attenuator knob set at 0.1, 0.2, 0.3 . . . turns (out of ten). The nesting heights of the peaks will tell you whether or not the system is behaving in a linear fashion. Continue to go higher on the 10-turn dial setting until you have visual evidence of saturation.

Once you have reached saturation, drop back into the linear range. Now you can operate with confidence that the signals you see really are proportional to the amplitude of the sound wave you are studying.

Experiment:

Set the hemispheres so that the scale angle $\alpha = 180°$.

Start the program SpectrumSLC.exe and measure an overview spectrum. You can use coarse steps such as 10 Hz and a short time per step such as 50 ms.

Change the angle between the upper and the lower hemisphere several times and observe the how the spectrum changes. Be sure to look at the spectrum for $\alpha = 0°$.

Question: What changes do you notice?

Experiment:

Go back to $\alpha = 0°$ and look in more detail at the peak near 5000 Hz. Actually, there are two peaks close to each other. Take a spectrum that measures slow enough and with sufficiently small steps to show the details of these two peaks. Also, take spectra for this range at $\alpha = 20°$ and $\alpha = 40°$.

Question: What do you notice?

Objective: Create polar plots for a series of resonances and use the plots to identify the angular momentum number and spherical harmonic function of each resonance.

Experiment:

Now we will measure the wavefunctions of the different resonances and visualize them by a polar plot of the amplitude $A(\theta)$. The computer calculates the polar angle θ from the angle α and it plots the absolute value of the amplitude as function of θ in a polar plot. This diagram makes it easy to identify the angular quantum number and the spherical harmonic function.

Take a spectrum with $\alpha = 180°$ from 2000 Hz to 7000 Hz sufficiently slowly. If you click with the left mouse button on a peak, the output frequency is adjusted to the value at which you clicked. Look at the oscilloscope and convince yourself that you are at a resonance. In the computer menu, go to “Windows” > “Measure Wave Function”.

Adjust the hemispheres to $\alpha = 0°$, and measure the amplitude in steps of 10°. The program converts the angle α automatically to the polar angle θ and plots the absolute of the amplitude in a polar plot. Use the function “complete by symmetry” to complete the figure.

Create polar-plots for the prominent peaks and identify the quantum numbers.

Analyze data:

Compare the polar plots you have generated with polar-plots of the Legendre polynomials. Some of them are given below, the others you can visualize with the program PlotYlm.exe.

In case of overlapping peaks, you will find distorted figures, since there are contributions to the wave functions from two different eigenstates with different quantum numbers and symmetries.

Fig. 2.3: Plots of the spherical harmonics:

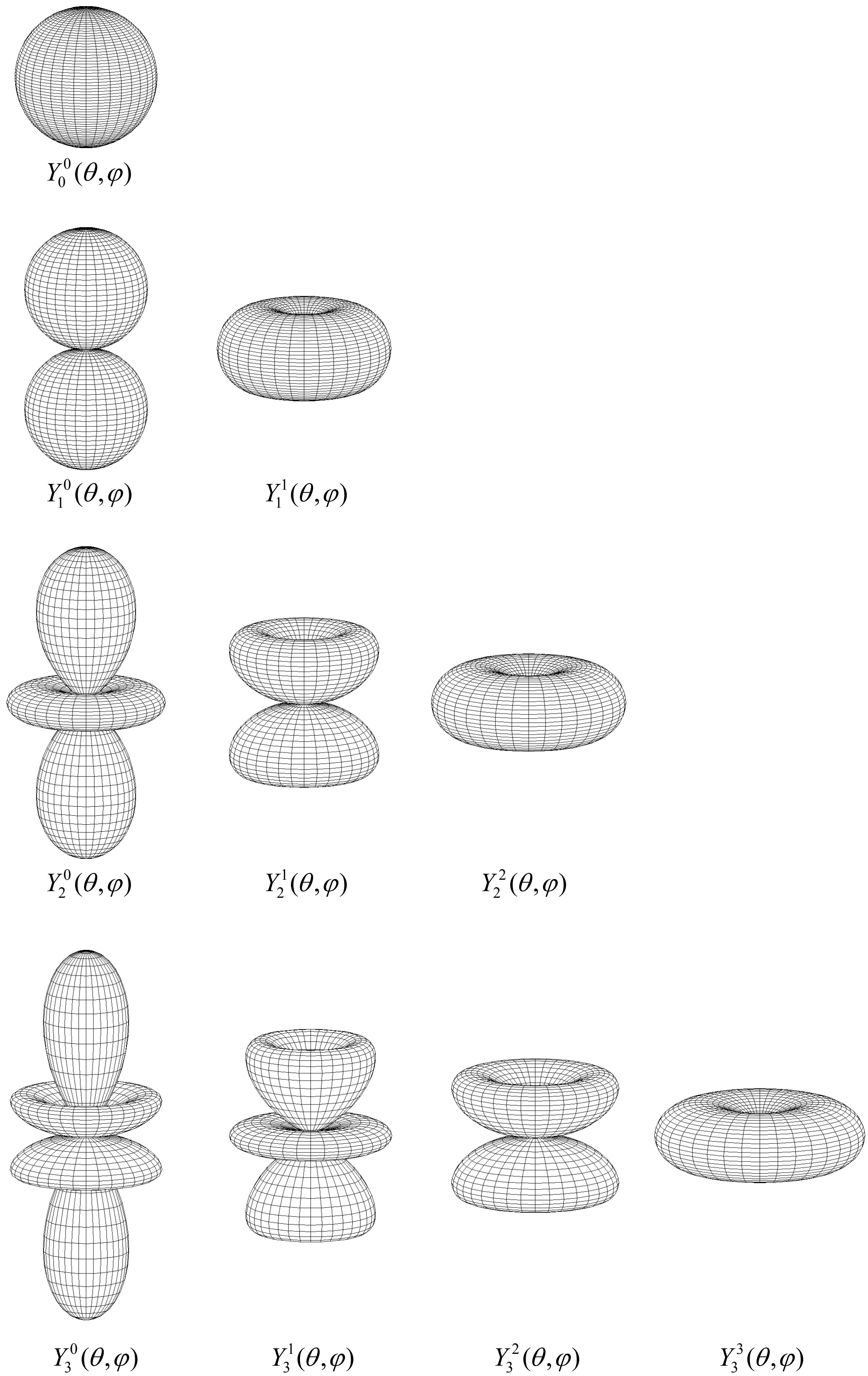
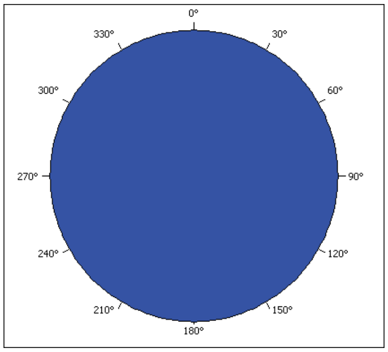
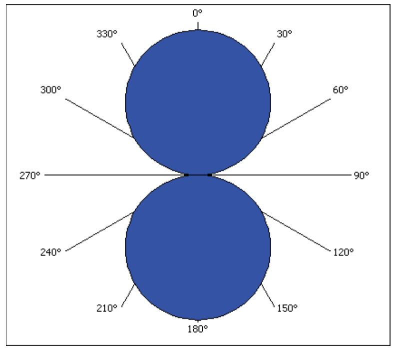


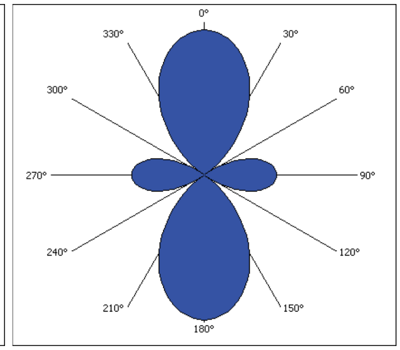
Fig. 2.4: Cut through the spherical harmonics with magnetic quantum number $m = 0$.



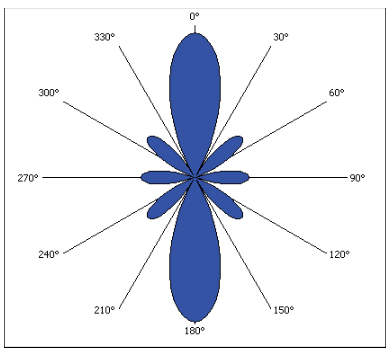
$Y_0^0(\theta,\varphi)$



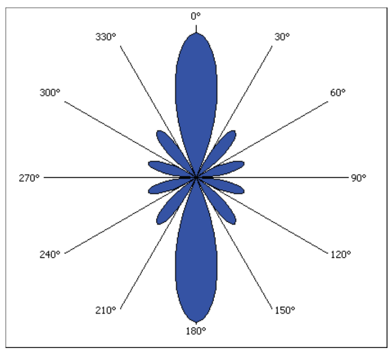
$Y_1^0(\theta,\varphi)$



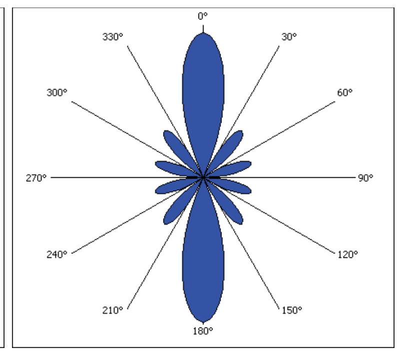
$Y_2^0(\theta,\varphi)$



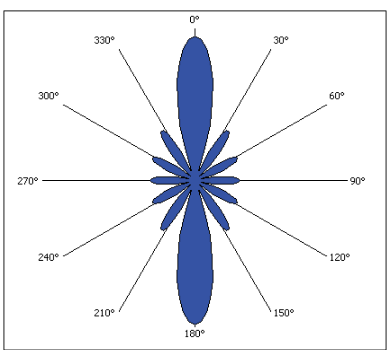
$Y_3^0(\theta,\varphi)$



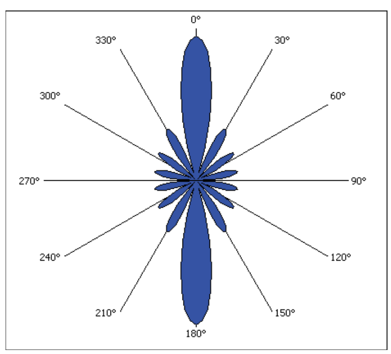
$Y_4^0(\theta,\varphi)$



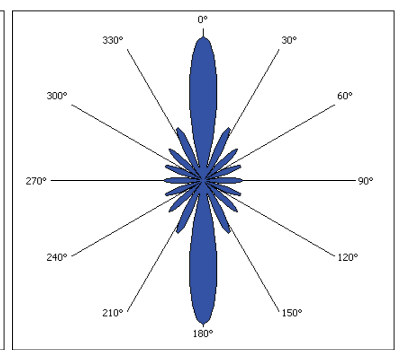
$Y_5^0(\theta,\varphi)$



$Y_6^0(\theta,\varphi)$



$Y_7^0(\theta,\varphi)$



$Y_8^0(\theta,\varphi)$

Quantum Analogs
Chapter 3
Student Manual

Broken Symmetry in the Spherical Resonator

and

Modeling a Molecule

Professor Rene Matzdorf
Universitaet Kassel

3. Broken symmetry in the spherical resonator and modeling a molecule

3.1 Lifting the degeneracy of states with different magnetic quantum numbers

Objective: In this series of experiments we will break the symmetry of the spherical cavity and study the resulting splitting of the resonance peaks. This is analogous to the splitting of quantum states.

Equipment Required:

TeachSpin Quantum Analog System: Controller, Hemispheres, Accessories
Computer with sound card installed and Quantum Analogs "SpectrumSLC.exe" running
Two adapter cables (BNC - 3.5 mm plug)
Two-Channel Oscilloscope

WARNING: The BNC-to-3.5-mm adapter cables are provided as a convenient way to couple signals between the controller and sound card. Unfortunately, they could also provide a way for excessive external voltage sources to damage a sound card. ***It is the user's responsibility to ensure that these adapter cables are NOT used with signals greater than 5 Volts peak-to-peak***. The maximum peak-to-peak value for optimum performance of the Quantum Analogs system depends on your sound card and can vary from 500 mV to 2 V.

Setup:

First, set the *ATTENUATOR* knob on the Controller at 0.2 (out of 10) turns.

Attach a BNC splitter to *SINE WAVE INPUT* on the controller. Using an adaptor cable, connect the output of your computer sound card to one side of the splitter. Use a BNC cable to send the sound signal to Channel 1 of the oscilloscope. Plug the lead from the speaker on the lower hemisphere to *SPEAKER OUTPUT* on the controller. The same sine wave now goes to both the speaker and Channel 1.

Use a BNC cable to connect the microphone output from the upper hemisphere to *MICROPHONE INPUT*. Connect *AC MONITOR* on the controller to Channel 2 of the oscilloscope to display the sound signal received by the microphone. Trigger the oscilloscope on Channel 1.

Important Note: You will need to adjust the magnitude of both the speaker and microphone signals to keep the microphone input to the computer from saturating. Refer to the Appendix titled 'Recognizing and Correcting Saturation' for instructions.

Experiment:

Measure a spectrum in the spherical resonator including only the lower three resonances.

Now put the 3 mm spacer ring between the upper and lower hemisphere. Measure the spectrum again. What do you observe?

Measure the spectrum again using the 6 mm spacer ring, and using both rings (9 mm).

Analyze the data:

For the $l = 1$ resonance, you can now plot the frequency splitting as function of spacer ring thickness. What relationship do you find?

Background:

In a spherical resonator, each resonance with angular quantum number l is $(2l+1)$-fold degenerate. These states with quantum numbers $m = -l, \ldots, 0, \ldots, l$ all have the same resonance frequency. In the spherical resonator, we have seen that the quantization axis (z-axis) is determined by the position of the speaker. The only wavefunction that has a non-zero amplitude on the z-axis is the one with $m = 0$. This is the reason why the $m = 0$ resonance is exited in the sphere, exclusively.

When a spacer ring is introduced, the spherical symmetry is broken and the degeneracy of the eigenstates is lifted. The quantization axis (z-axis) is now determined by the symmetry axis of the resonator, which is the vertical axis. The speaker, which has a θ=45° position with respect to the symmetry axis, can now excite all states with different quantum numbers m. The sketch in Figure 3.1 will help you to visualize the direction of the quantization axis.

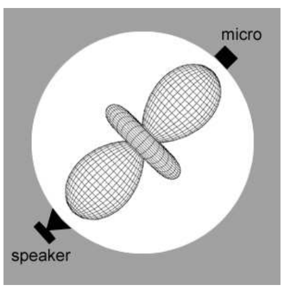
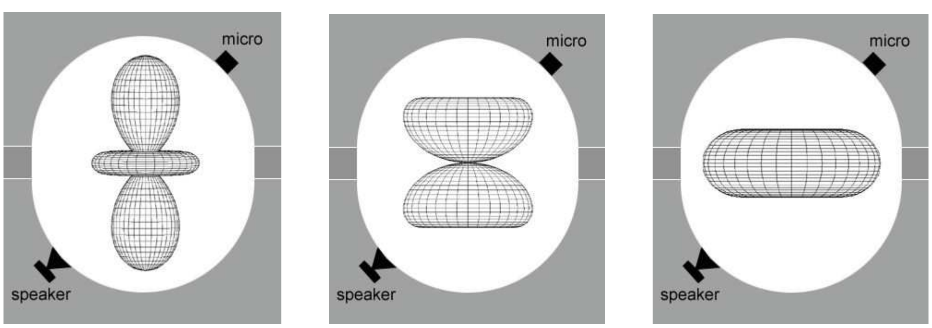


Fig. 3.1a: In the spherical resonator, the quantization axis is determined by the position of the speaker because it is the only part that breaks symmetry.



$m = 0$ $m = 1$ $m = 2$

Fig. 3.1b: In the resonator elongated by spacer rings, the quantization axis is given by the symmetry axis of the resonator. The degeneracy of the states with different m is lifted.

The degeneracy is not lifted completely because the states with positive and negative magnetic quantum number $\pm m$ are still degenerate. States with positive and negative m belong to waves in the resonator circulating around the quantization axis in right-handed and left-handed directions, respectively. Both of these waves are excited by the speaker and have the same amplitude for each m. A superposition of such two waves results in a standing wave with respect to the azimuthal angle φ.

$$e^{im\varphi} + e^{-im\varphi} = 2\cos(m\varphi) \tag{3.1}$$

In quantum chemistry, the superposition of the positive and negative versions of the magnetic quantum number m is used to form orbitals. Examples of the way these are labeled are: p_x, p_y, d_{xz}, d_{yz} for m=1 and d_{xy}, $d_{x^2-y^2}$ for m=2.

In the sense of perturbation theory, the eigenfunctions in broken symmetry are modified only slightly compared to the eigenfunctions of the spherical symmetric case, as long as the perturbation is small. We can therefore expect wavefunctions very similar to the spherical harmonics.

In the next experiments you can measure the azimuthal dependence of the wavefunctions and identify the magnetic quantum number of the peaks.

Experiment:

Using in turn the 3 mm, 6 mm and 9 mm spacer rings, acquire a high-resolution spectrum of the l = 1 resonance that resolves the two peaks attributable to m = 0 and m = ±1.

Experiment:

Now we will measure the amplitude as function of the azimuthal angle φ. We will then identify which m belongs to each peak. Click the left mouse button on top of a peak to choose this particular frequency. Then, open the window to measure the wavefunction (→ Windows → Measure Wave Function). Check the box labeled "Lifted degeneracy" to tell the program that the quantization axis is now vertical and that the angle α on the scale is equal to the azimuthal angle φ. In this mode the wavefunction is displayed in green.

Now you can measure the amplitude of the peak as function of azimuthal angle φ. Repeat the same measurement for the other peak. Use the oscilloscope to determine how changing the azimuth angle affects the sign of the microphone signal.

Alternatively, you can measure the amplitude by hand. Read the amplitude from the oscilloscope and the azimuthal angle φ = α from the scale.

Analyze the data:

Identify the magnetic quantum number for each of the peaks. Compare your results for the amplitude as function of φ with the theoretical prediction $A(\varphi) = \cos(m\varphi)$.

Experiment:

Choose the frequency of the $l = 1$ and $m = 0$ resonance and measure the phase of the microphone signal in the upper hemisphere at $\alpha = 180°$. Then, connect the cable to the microphone in the lower hemisphere and measure the phase again. Repeat the same experiment with the $m = 1$ resonance.

Experiment:

Measure a highly resolved spectrum with 3 mm, 6 mm and 9 mm spacer rings of the $l = 2$ resonance. It will split into three peaks with $m = 0$, $m = \pm 1$ and $m = \pm 2$.

Experiment:

For each of the three peaks, measure the amplitude as function of azimuthal angle φ and identify the magnetic quantum numbers.

Experiment:

You may measure the splitting of states with higher *l,* but the increasing overlapping of several peaks with different magnetic quantum number makes an identification of *m* more and more difficult.

One possible way to overcome this problem is to measure spectra for all angles φ and use the peak fitting procedure to determine the peak amplitudes. With this technique the overlapping of the peaks becomes irrelevant.

Another possibility is to measure at certain angles φ for which nodes in the wavefunction are expected for particular magnetic quantum numbers. If one of the peaks in the spectrum disappears at the nodes of a certain magnetic quantum number, its number has been identified.

3.2 Modeling a molecule

Objective: We will use a pair of spheres to create an analog of a hydrogen molecule.

Equipment needed:

TeachSpin Quantum Analogs System: Controller, 4 hemispheres, irises
Computer with sound card installed and Quantum Analogs "SpectrumSLC.exe" running
Two-Channel Oscilloscope
Two BNC – 3.5 mm plug adaptors

Setup:

Set a hemisphere with a hole on top of the hemisphere with the speaker. Through this hole, the sound in the lower sphere will couple to a second sphere. The strength of the coupling can be adjusted by choice of the iris diameter. Choose one of the irises and put it in place. (Iris diameters are 5 mm, 10 mm 15 mm or 20 mm.) Set the hole in the next hemisphere against the iris. Use the hemisphere with the microphone to complete the upper sphere.
Put BNC splitters on both the *SINE WAVE INPUT* and the *AC-MONITOR* of the controller box. Using a BNC to 3.5 mm jack converter, connect the output of the computer's sound card to one side of the BNC splitter on *SINE WAVE INPUT*. Connect the other side to Channel 1 of the oscilloscope. Connect the speaker cable from the lower hemisphere to *SPEAKER OUTPUT* on the controller. (The sound card signal now goes to both the speaker and the 'scope.)

Use a BNC cable to connect the microphone in the top-hemisphere to *MICROPHONE INPUT*. Use a BNC cable to send the microphone signal from one side of the splitter on *AC-MONITOR* to Channel 2 of the oscilloscope. Use an adaptor cable to connect the other arm of the splitter on *AC-MONITOR* to the microphone line-in of your sound card.

Important Note: You will need to adjust the magnitude of both the speaker and microphone signals to keep the microphone input to the computer from saturating. Refer to the Appendix titled 'Recognizing and Correcting Saturation' for instructions.

Experiment:

Measure a spectrum in the "molecule" (two coupled spherical resonators) of the resonance at 2300 Hz. Repeat the measurement with the different irises. Compare with a measurement of this peak in the "atom" (spherical resonator).

Open questions:

Why does the peak split?

What is lifting the degeneracy?

Which quantum numbers can we use to label the peaks in the molecule?

What do the molecular orbitals look like?

Let's answer these questions step by step.

Experiment:

Measure a spectrum in the frequency range from 0 Hz to 1000 Hz first in the "atom" and then in the "molecule". Repeat the measurement with the other irises.

Analyze the data: Make a plot of the resonance-frequency as function of iris diameter.

Experiment:

Use one of the bigger irises and choose exactly the frequency of the resonance. This can be done by clicking the left mouse-button on the top of the peak. For the upper sphere, measure the phase of the microphone signal (*AC-MONITOR* connected to Channel 2 of the oscilloscope) with respect to the *SINE WAVE INPUT* signal (Channel 1 of the oscilloscope). Now connect the microphone in the lower sphere to the amplifier and repeat the measurement.

Question:

What is the phase difference between upper and lower sphere?

Experiment:

In the upper sphere, you can measure the azimuthal dependence of amplitude to identify the symmetry of the wavefunction.

:

Background:

The two, coupled spherical resonators model a diatomic molecule with two identical nuclei, a so-called homonuclear diatomic molecule. The simplest example of such a molecule is H_2^+. Since this molecule has only one single electron moving in the potential of two protons, it is an ideal model system to discuss quantum mechanical effects in molecules. Many of the observations can be transferred to molecules like H_2, O_2, N_2 and F_2.

Diatomic molecules have cylindrical symmetry with respect to the axis going through the nuclei. Due to this symmetry, we expect that *m* is a good quantum number for the molecule, just as it is in the atom. The quantum number *l*, however, cannot be used in molecules. In the sense of perturbation theory, we expect a continuous change from the atomic orbitals into the molecular orbitals as function of the nuclear distance. We will therefore label the molecular states additionally by the atomic states from which they are derived in square brackets (for example: $1\sigma_u$[1s]).

For a small coupling of the two atoms (a large inter-nuclear distance), a superposition of atomic orbitals is a fairly good approximation for the molecular orbitals. In general, the two atomic orbitals can be superimposed in two different ways to produce a molecular orbital: with the same sign or with different signs (phase shift 180°). Depending on the sign, the molecular orbital is labeled with an index: g for the German word gerade = even, when the signs are the same and u for the German word ungerade = odd, when the signs are different.

The quantum number m is labeled with Greek letters σ, π, and δ for *m* = 0, *m* = 1, and *m* = 2, respectively. This corresponds to the way the Latin letters s, p, d are used in the atom for the quantum number *l*. Additionally, a principal quantum number is used to number states with the same symmetry but with increasing energy. In this sense, the state $1\sigma_u$[1s] describes a molecular orbital derived from two 1s atomic states that have been superimposed with different sign. It has the magnetic quantum number m = 0 and is the first state with this symmetry.

In the following figure, the molecular orbitals derived from 1s states are plotted.

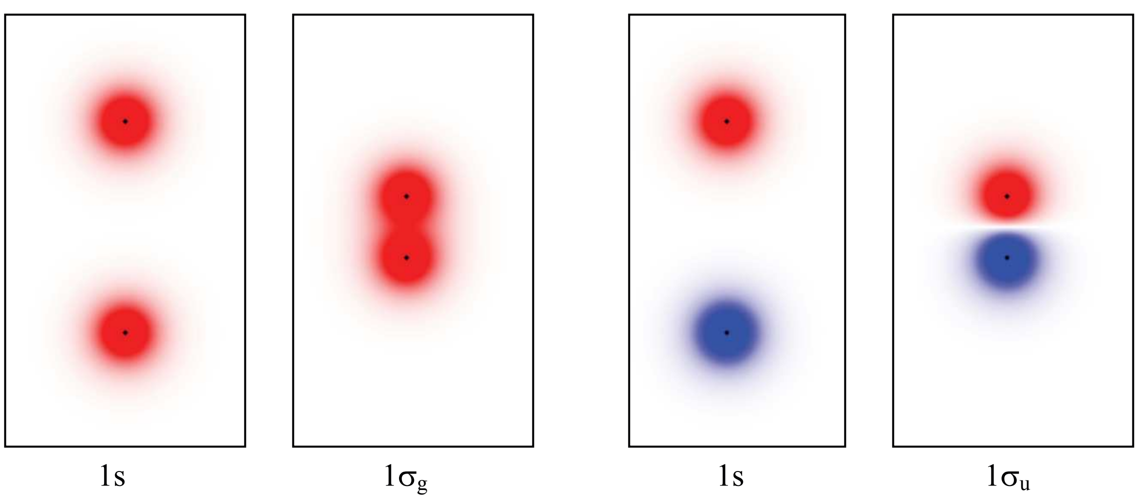


Fig. 3.2: Atomic 1s orbitals for two atoms with large distance and corresponding molecular orbitals calculated by superposition of 1s atomic orbitals.
The color indicates the sign: red = positive, blue = negative

Molecular orbitals with a high probability of finding the electron between the two nuclei are called bonding states, because they form a molecular bond. States that have a node between the nuclei, resulting in much lower electron density between the nuclei, are called anti-bonding. If they are occupied by electrons, it weakens the bond strength between two atoms. In the case shown in Fig. 3.2, as in most cases, the even state $1\sigma_g$[1s] is bonding and the odd state $1\sigma_u$[1s] is anti-bonding.

What is analogous, what is different?

In the acoustic analog, we have a situation very similar to that of the real molecule. The two, coupled spheres with same diameter correspond to the two identical nuclei that are coupled through the iris between them. The diameter of the iris determines the coupling strength, which corresponds to the internuclear distance of the real molecule. The symmetry is cylindrical, as it is in the real molecule. Therefore, we can use the same quantum numbers and labeling of states as in the real molecule. Due to different boundary conditions, and the absence of a potential, the eigenstates have a different order than in real molecules. The eigenstates can be identified experimentally by the "atomic" states from which they are derived by the quantum number *m* and by the phase of the wave function in the two spheres.

The eigenstate with a wave function that has no node at all (equal phase everywhere in space) has the frequency zero in the acoustic case. This is due to Neuman's boundary conditions that would result, for this case, in a constant amplitude of pressure everywhere. It cannot oscillate. In the case of a molecule this state is the $1\sigma_g$[1s] state, the ground state of the H_2^+-molecule. It cannot be observed as resonance in the acoustic analog.

The state with lowest frequency in the acoustic analog is the $1\sigma_u$[1s]. It is derived from 1s states of the uncoupled "atoms", even though the 1s states of the uncoupled atoms cannot be observed because, for both, the frequency is zero. With increasing coupling strength, the frequency of this state increases, as you observed in the experiment above. Since the state is odd, the phase of the wave function has different sign in both spheres. You observed this on the oscilloscope when you measured the signal at the two different microphone locations in the two spheres. The state is a σ-state since the amplitude is constant as function of $\varphi = \alpha$ as you observed by rotating the top hemisphere. For higher *m*, the amplitude would show a dependence as $\cos(m\varphi)$.

π and δ orbitals

From atomic *p* orbitals, we derive molecular orbitals that can have magnetic quantum numbers $m = 0$ (σ) and $m = 1$ (π). Due to even and odd superposition, this results in four different molecular orbitals: σ_g , σ_u, π_g , π_u . In the case of atomic d-orbitals the number of derived molecular orbitals is six: σ_g , σ_u, π_g , π_u, δ_g , δ_u . The following figure shows the molecular orbitals along with the atomic orbitals they are derived from.

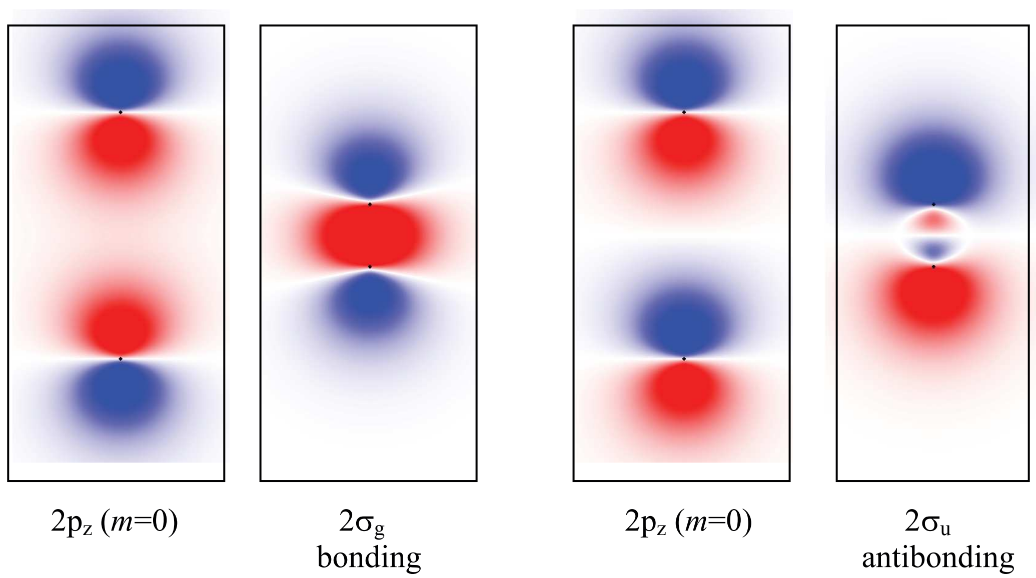


Fig. 3.3a: Molecular σ-orbitals derived from the atomic 2p-orbital.

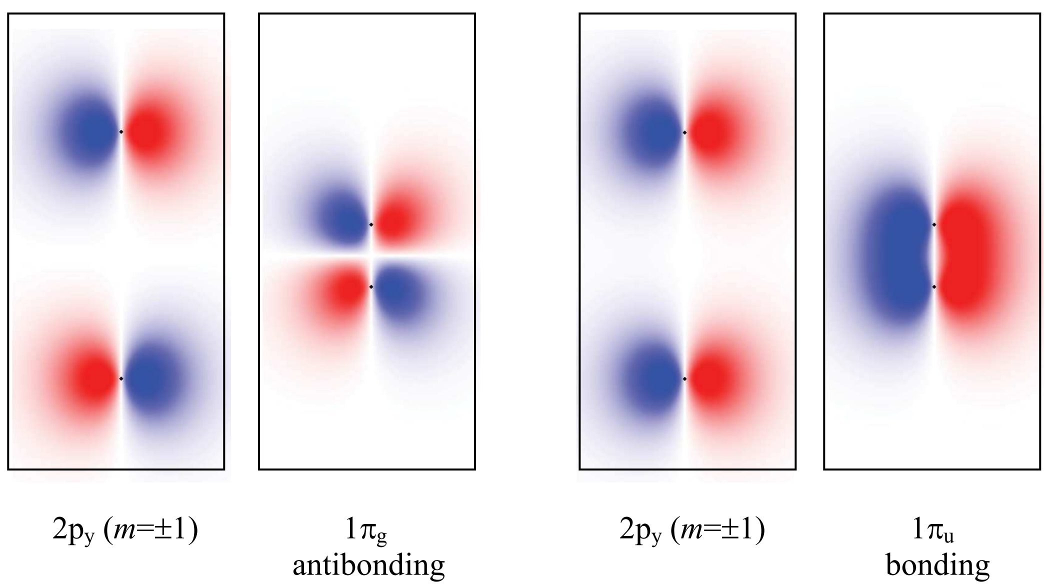


Fig. 3.3b: Molecular π-orbitals derived from the atomic 2p-orbital.

Experiment

Let us now investigate the molecular orbitals derived from the first atomic p-state that is observed at about 2300 Hz.

Measure a resonance spectrum in the “atom” for reference and then take a measurement in the “molecule”. Use the 20 mm iris to produce the maximum splitting of the peaks.

Before measuring, press down firmly on top of the pile of hemispheres. Good contact is necessary to resolve peaks that are close to each other. You should scan slower than 50 ms/Hz.

Take spectra at different azimuthal angles.

Experiment

Now we want to identify the peaks in the spectra. In addition to the peak at about 2450 Hz there are *three peaks* around 2300 Hz, even though it looks like a double-peak structure.

You can measure the phase difference between the upper and lower spheres for the different peaks. Note that it is only in the $\alpha = 180°$ position that the microphone positions are equivalent for the upper and lower hemisphere. For all other α, you have to take the azimuthal dependence into account.

In the case of strongly overlapping peaks, it is difficult to measure the phase directly. Here you may observe how the amplitude develops as function of azimuth.

Quantum Analogs
Chapter 4
Student Manual

Modeling a
One Dimensional Solid

Professor Rene Matzdorf
Universitaet Kassel

4. Modeling a one-dimensional solid

There are two different ways to explain how a band structure in a periodic potential of a solid develops. One approach starts with a free moving electron in a constant potential that has a parabolic dispersion relation E(k). Introducing periodic scattering centers with small reflection probability results in the opening of band gaps. The other approach is to start from an atom with its discrete states. The next steps in this approach are the splitting of the eigenstates states in a two-atom molecule and further splitting in a chain with *n* atoms. With the acoustic analog, you can study both approaches experimentally. We will do this in the next two sections. In later sections, we will model the electronic structure in more complex solids with superstructures (Section 4.3) and defects (Section 4.4).

4.1 From a free electron to an electron in a periodic potential

To model a free electron in one dimension, we are using propagating sound in a tube. Since we cannot work with infinitely long tubes, we restrict ourselves to a finite tube with hard walls on both ends. This is actually the same setup we used in Chapter 1 to model the "particle in a box". Due to the finite length *L* of the tube we get resonances with the frequencies *f* :

$$f_n = n\frac{c}{2L} \tag{4.1}$$

(*c* is the speed of sound and *n* is an integer number n=1,2,...∞). The longer the tube, the denser the resonances become. In an infinitely long tube, the resonances would be infinitely dense. In solid-state physics, the so-called "density of states" is used in this context. Now let's do an experiment.

Equipment Required:

TeachSpin Quantum Analog System: Controller, V-Channel & Aluminum Cylinders, Irises
Two-Channel Oscilloscope
Two adapter cables (BNC - 3.5 mm plug)
Computer with sound card installed and Quantum Analogs "SpectrumSLC.exe" running

Setup:

First, set the *ATTENUATOR* knob on the Controller at 0.2 (out of 10) turns

Using the tube-pieces, make a tube with the end-piece containing the speaker on one end and the end-piece with the microphone on the other. Attach a BNC splitter to *SINE WAVE INPUT* on the controller. Using the adapter cable, connect the output of the sound card to one arm of the splitter. With a BNC cable, convey the soundcard signal from the splitter to Channel 1 of your oscilloscope. Plug the lead from the speaker end of your experimental tube to *SPEAKER OUTPUT* on the controller. The sound card signal is now going to both the speaker and Channel 1.

Connect the microphone on your experimental tube to *MICROPHONE INPUT* on the controller. Put a BNC splitter on the controller connector labeled *AC-MONITOR*. From the splitter, use an adapter cable to send the microphone signal to the microphone input on the computer soundcard and a BNC cable to send the same signal to Channel 2 of the oscilloscope. Channel 2 will show the actual signal coming from the microphone.

The computer plots the instantaneous frequency generated by the sound card on the x-axis and the amplitude of the microphone input signal on the y-axis. Configure the computer so that "microphone" or "line-in" is chosen as the input

You will need to adjust the magnitude of both the speaker and microphone signals to keep the microphone input to the computer from saturating. (*It is the user's responsibility to ensure that the adapter cables are NOT used with signals greater than 5 Volts peak-to-peak.*)

Refer to the Appendix titled 'Recognizing and Correcting Saturation' for instructions.

Experiment:

Measure the resonances in tubes of different length and analyze the distance between the resonances $\Delta f = f_{n+1} - f_n$ as function of tube length. Convince yourself that the resonances become more and more dense with increasing tube length. (As you use longer tubes, you will to increase the *ATTENUATOR* setting in order to get good data.)

The quantum numbers used in solid-state physics are different from those used in atomic and molecular physics. In the measurements you have made, you will have noticed that there are equidistant resonances, which can be characterized by numbering them in the order of their frequency. From theory, we know that they belong to standing waves in the tube with wavelength

$$\lambda = \frac{2L}{n} \qquad (4.2)$$

The wavelength can also be expressed by another quantity called "wave number" k (in three dimensions it is the "wave-vector", $\vec{k}$).

$$k = \frac{2\pi}{\lambda} = n\frac{\pi}{L} \qquad (4.3)$$

In the case of infinitely dense eigenstates, it is not useful to number the states by an integer number. It is better to use the wave-number k (or wave-vector $\vec{k}$ in higher dimensions) to label the eigenstates. In atomic physics we have characterized the quantum mechanical system by energies $E(n,l,m)$ as function of integer quantum numbers, in solid-state physics the quantum mechanical system is characterized by the energy $E(k)$ as function of wave number. This relation is called "dispersion relation". We will do this analogously in the acoustic experiments.

In the tube with finite length, we have discrete eigenstates, so that it is easy to determine the wave number by the index n of the resonance using eqn. 4.3. This now allows us to measure the dispersion relation for a sound wave in an empty tube.

Experiment:

Measure the frequencies of the resonances in a tube of length L = 600 mm and plot the frequency as function of wave number k.

What do you notice?

What is analogous, what is different?

Sound waves show a linear dispersion with a slope proportional to sound velocity.

$$f(k) = \frac{c}{2\pi} k \tag{4.4}$$

Electrons, however, have a parabolic dispersion

$$E(k) = \frac{\hbar^2}{2m} k^2 . \tag{4.5}$$

Modifications of this so called free-electron like dispersion are observed, when electrons have a wavelength that is comparable to twice the lattice constant, *a*, of the solid. In this case, the electrons are scattered effectively by the periodic lattice.

In the acoustic analog, we introduce periodic scattering centers separated by a distance, *a*, that is comparable to half the wavelength of sound. A typical wavelength, at reasonable frequency, (3.4 kHz) is λ = 10cm (≈4 inch). Therefore, we can model a lattice by periodic scattering centers at a separation distance of about *a* = 5cm (≈2 inch).

Experiment:

Take an overview spectrum (0-12 kHz) of a tube made from 12 tube-pieces each 5 cm long.

Now, insert 11 irises with an inner diameter of 16 mm between the pieces and measure a spectrum again.

What do you observe?

Due to the introduction of the periodic scattering sites, a band structure has developed. It shows bands and band-gaps. Because we have a tube with a finite length, the bands consist of discrete resonances. The band-gaps indicate frequency ranges in which no sound can propagate through the periodic structure.

Experiment:

Remove the end-piece with the microphone and put your ear in its place.

Choose a frequency within a band. Then choose a frequency within a band gap. Listen to the difference in loudness.

Now we want to study how the spectrum is influenced by a variety of parameters (Diameter of the irises *d*, number of pieces *j* and length of a tube-piece *a*).

Experiment:

Replace the end-piece and measure spectra with irises of 13 mm and 10 mm diameter.

Now we will measure spectra for a different number of unit cells. In solid-state physics, a “unit cell” is the part of space that is repeated periodically to build up the solid. In our case, it is the combination of a tube-piece and an iris. We have not put a 12^{th} iris in front of the microphone, since the end-piece reflects the sound perfectly, anyway. You may convince yourself that the use of a 12^{th} iris at one of the end-pieces makes no significant difference in the spectra. Small changes are due to the amount of air within the hole of the iris. For future experiments, you may decide for yourself whether to put an iris at an end-piece.

Experiment:

Put in the 16 mm irises again and measure spectra for different numbers of tube-piece / iris .

Describe the way the spectrum changes. Are there any mathematical patterns?

Now let’s study how the spectrum depends on the length of a tube-piece *a*, which corresponds to the lattice constant in solid-state physics.

Experiment:

Take a spectrum with 8 pieces 50mm long and irises of 16mm diameter. Than replace the 50 mm long pieces by 75 mm long pieces. What difference in the spectra do you observe? Can you find a mathematical pattern?

Background information:

Band gaps open up when the "Bragg condition" is fulfilled. Probably you know the Bragg condition from x-ray and neutron scattering at crystals, which are both examples of wave reflection at a periodic lattice. The Bragg conditions is fulfilled, when

$$n\lambda = 2a \tag{4.6}$$

(a is the distance of reflecting planes). In our one-dimensional case the reflecting irises represent the reflecting planes of a solid. Reflection in the solid is so effective at this wavelength since the reflected waves from each plane add up constructively with perfectly fitting phase. This is the reason why waves cannot propagate easily at this wavelength.

A very convenient way to describe the scattering phenomena at periodic structures is to use the so-called "reciprocal space". The reciprocal space is the space of the wave vectors $\vec{k}$. In our one-dimensional case we have a one-dimensional reciprocal space with the wave-numbers k. If a wave is reflected at a periodic structure and the Bragg condition is fulfilled and the wave number $\vec{k}$ has changed to $\vec{k}'$, then the difference $\vec{k}' - \vec{k} = \vec{G}$ is called a "reciprocal lattice vector" $\vec{G}$. In our one-dimensional case the wave has been reflected and k has changed to $-k$ with a k that fulfils the Bragg condition.

$$k = n\frac{\pi}{a} \tag{4.7}$$

In consequence, the reciprocal lattice vectors for the one-dimensional case are given by

$$G = n\frac{2\pi}{a} \tag{4.8}$$

with an integer number n that can be positive or negative or zero. In general, the reciprocal lattice vectors are forming a periodic lattice in the reciprocal space, which is called the "reciprocal lattice". In this reciprocal lattice you can define unit cells of the reciprocal space that are called "Brillouin zones". For the one-dimensional case the reciprocal lattice points and the Brillouin zones (BZ) are displayed in Fig. 4.1.

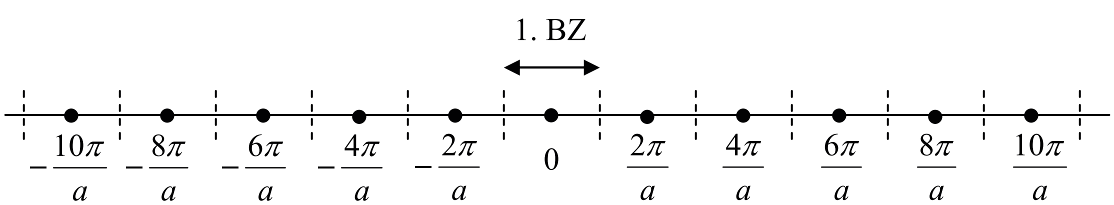


Fig. 4.1: Reciprocal lattice points (black dots), and Brillouin zones boundaries marked by dashed lines.

Due to the finite length of the tube we have discrete k-points in the reciprocal at which an eigenstate (resonance) is observed. They are given by eqn 4.3. If we compare the smallest reciprocal lattice vector

$$G = \frac{2\pi}{a} \tag{4.9}$$

with the distance of the discrete k-points in the tube of finite length L

$$k = \frac{\pi}{L} \tag{4.10}$$

we can see that there are $2L/a$ discrete k-points in each Brillouin zone. Since $L = j \cdot a$ we can conclude that the number of discrete k-points in a Brillouin zone is twice the number of unit cells. At k=0 and zero frequency (energy) there is no resonance (eigenstate) for a finite system.

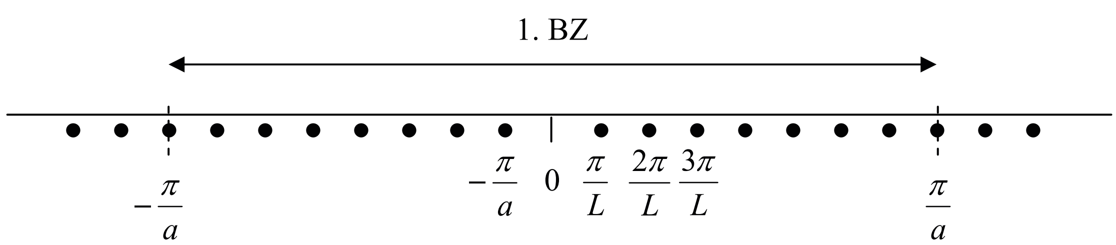


Fig. 4.2: Discrete k-points in reciprocal space (black dots), and first Brillouin zone marked by dashed lines. The example represents a setup with 8 unit cells.

Let us now explore the dispersion relation in reciprocal space.

Analyze the data:

Plot the frequency as function of wave number for resonances in a setup made from 8 pieces 50 mm long and 7 irises of 16 mm diameter.

Determine the wave number as given in eqn. 4.3.

Where, in reciprocal space, do the band gaps open up?

When counting the resonances, please note that the little peak at 370 Hz is **not** a resonance. It is a peak in the transmission function of the speaker/microphone combination.

Background Information

From Bloch's theorem, we know that wave functions in a periodic structure can be written as the product of a function $u_k(x)$ that has the periodicity of the lattice and exp(i*kx*) with the periodicity given by the wave number.

$$\psi(x) = u_k(x)e^{ikx} \qquad (4.11)$$

A function of this form can be written in the form

$$\psi(x) = \sum_G C_{(k-G)} e^{i(k-G)x} \ . \qquad (4.12)$$

From this form of notation, we see that the wave function cannot be assigned to a single point in the reciprocal space. The wave function is a sum with contributions from a single k-point in each Brillouin zone. All of these k-points are connected by reciprocal lattice vectors. In solid-state physics, therefore, the dispersion $E(k)$ is usually plotted only in the first Brillouin zone. This is called the "reduced zone scheme" in contrast to the "extended zone scheme".

Analyze the data:

Plot the dispersion relation $E(k)$ in the reduced zone scheme

Analyze the data:

Analyze the spectra for a setup made from 10 unit cells with 50 mm tubes and 16 mm irises and for a setup made from 12 unit cells with 50 mm tubes and 16 mm irises.

Plot the dispersion relation into the reduced zone scheme. Note that at higher frequencies, the first and the last resonance in a band cannot be identified easily.

You should keep in mind that each band has j resonances when it is build up from j unit cells. Only the first band has j-1 resonances because the lowest state of that band has zero frequency and is not visible. This is important when you determine the wave number from the resonance number n.

Analyze the data:

Analyze the spectra for a setup made from 8 unit cells with 75 mm tubes and 16 mm irises and compare it to a setup made from 8 unit cells with 50 mm tubes and 16 mm irises.

Plot the dispersion relation into the reduced zone scheme.

Analyze the data:

Analyze the spectra for a setup made from 8 unit cells with 50 mm tubes and 16 mm, 13mm and 10 mm irises, respectively.

Plot the dispersion relations into the reduced zone scheme.

How does the dispersion depend on the iris diameter?

In condensed matter physics, the density of states (DOS) is often discussed. If the dispersion relation is known in the complete Brillouin zone, the DOS can be calculated from these data. To illustrate how the DOS of a one-dimensional system looks, we will now analyse the data with respect to this quantity.

Analyze the data:

Let's take the spectrum for a setup made from 8 unit cells with 50 mm tubes and 16 mm irises and use it to determine the DOS. Since this is a system with a small number of unit cells, we cannot simply count the number of states within an energy interval. We will therefore calculate the density by one over the frequency distance between two states.

$$\rho(f) \approx \frac{1}{f_{i+1} - f_i} \tag{4.12}$$

In a one-dimensional band structure, there are singularities in the density of states expected at the band edges (van Hove singularity), since the slope of the bands approaches zero at zone boundaries and symmetry planes. Due to the finite number of unit cells, the density of states is finite in our experiment, but a significant upturn of DOS at the band edges is clearly visible.

4.2 Atom – Molecule – Chain

In the previous section, we have seen how band-gaps develop in a free moving wave when periodic scattering sites are introduced. The other approach to solid-state physics starts with the eigenstates of a single atom. When two atoms are combined into a molecule, a splitting of the eigenstates into bonding and anti-bonding states is observed. Finally, bands develop from these levels, when many atoms are arranged into a chain. In theory, this approach is called the tight binding model. Now we want to study this approach experimentally starting with an atom, which we will model with a 50 mm long cylinder with the speaker on one end and the microphone on the other.

Experiment:

Take an overview spectrum (0-22 kHz) in a single 50 mm long tube-piece.

The peaks at 370 Hz, 2000 Hz and 4900 Hz are not resonances in the tube. They are due to the frequency response of the speaker and microphone combination, which is not frequency independent. Below 16 kHz there are 4 resonances in the 50 mm long cylinder, which can be described as standing waves with 1, 2, 3 and 4 node-planes perpendicular to the cylinder axis, respectively. At frequencies above 16 kHz, resonances are observed that have radial nodes (cylindrical node surfaces). The inner diameter of the tube, which is 25.4 mm (1 inch), determines the frequency of the first radial mode. In the following, we want to concentrate on the resonances below 16 kHz (longitudinal modes). For these states, the magnetic quantum number m is zero (σ-states).

Experiment:

Measure a spectrum in a longer tube-piece (75 mm). You will see that the resonances of the longitudinal modes shift down in energy, but the first radial mode stays above 16 kHz.

The next step is to model a molecule by combining two pieces of 50 mm long tube with an iris of 10 mm diameter (Ø10mm) between them. We are choosing to use the smallest iris because we want to model a weak coupling of the atoms.

Experiment:

Take a spectrum (0-12 kHz for example) in a combination of two 50 mm long tube-pieces with an iris Ø10 mm between them. What do you observe?

Note that the lowest bonding state has the frequency zero. The first antibonding state is observed at about 1100 Hz. For the other peaks the splitting in bonding / antibonding states is visible clearly. Remember that the small peaks at 370Hz and 2000Hz are due to the frequency response of speaker and microphone.

Experiment:

Repeat the experiment with Ø13 mm and Ø16 mm irises. What is different?

Experiment:

Take spectra with an increasing number of unit cells and observe how bands develop.

Analyze data

Compare the frequency difference between bonding and antibonding states with the width of the corresponding band in a setup with large number of unit cells.

4.3 Superstructures and unit cells with more than one atom

In this section, we will study the band structure of a periodic lattice that has a more complicated periodicity. A superstructure is a periodic perturbation of a periodic lattice. The periodic perturbation has a translation vector that is an integer multiple of the original lattice vector. This can be, for example, a modification of every second unit cell. A superstructure results in a new periodicity with a larger lattice vector, smaller Brillouin zone and a smaller reciprocal lattice vector. There are many fields in condensed matter physics where superstructures play an important role. For example, in surface science many surface structures show a superstructure with respect to the bulk lattice. Another well-known example for a superstructure in a bulk lattice is a Peierls distortion. We will study the effect on band structure by introducing a periodic perturbation into our one-dimensional lattice.

Experiment:

Make a setup of 12 tube-pieces 50 mm long and 13 mm irises and measure a spectrum. Then, replace every other iris by a 16 mm iris and measure the spectrum again. What do you observe? Plot the band structure for both cases.

Experiment:

Make a setup of 5 unit cells with each unit cell made of a 50 mm tube, a 16 mm iris, a 75 mm tube, and 16 mm iris. Measure a spectrum and plot the band structure.

Experiment:

We want to understand this band structure better by using the tight binding model and compare therefore the energy levels with the resonances found in the single “atoms”. Take spectra in a 50 mm tube and in a 75 mm tube. Compare the “atomic” levels with the band structure. What can you conclude? You may also compare to a spectrum measured in a single unit cell.

Experiment:

You may now build different superstructures by yourself and try to understand the change in band structure due to the new periodicity.

4.4 Defect states

In this section we will see how defects change the band structure. Defects destroy the periodicity of the lattice. They are localized perturbations. If the defect density is small, the band structure is more or less conserved and additional states are introduced due to the defects. The most important example for such defects states in condensed matter physics is certainly the doping of semiconductors. The introduction of defect-states creates the acceptor and donator levels that are responsible for the unique properties of these materials.

Experiment:

Make a setup of 12 tube-pieces 50 mm long and 16 mm irises and measure a spectrum.

Then, replace one tube-piece by a 75 mm long piece and measure the spectrum again. What do you observe?

Plot the band structure for both cases.

Note that the defect-state that is observed in the first band-gap has a localized wavefunction. Since it is localized, it cannot be assigned to a sharp wave-number. The state is therefore plotted as a horizontal line into the band structure in order to indicate that it has no well-defined wave-vector. You may have noticed that the peaks within the upper bands have shifted a little bit and no longer show the high regularity they did without defect. This is due to the fact that the lattice has lost its periodicity and, strictly speaking, it is no longer allowed to use the wave-number as a good quantum number. However, from the plot of the band structure you see that the defect does not change the band structure significantly. We can treat it as a small perturbation and use the reciprocal space with the Brillouin zone as we did in the periodic lattice.

Experiment:

Put the defect at other positions within the one-dimensional lattice and measure the spectra produced. Does the frequency of the defect-resonance depend on the position?

Experiment:

Use other tube lengths as a defect. You can try 25 mm, 37.5 mm and 62.5 mm for example.

In some cases you find the defect state close to a band edge. Such a situation is used in doped semiconductors. Donor-levels are defect states that are occupied by electrons and have a position just below the conduction band. The electrons can be excited easily into the conduction band and move there freely. This is very similar our case with a 62.5 mm tube as a defect. Acceptor-levels are unoccupied defect states just above the valence band. Electrons can be excited easily from the valence band into the defect states and the remaining holes in the valence band are responsible for the conductivity.

Further experiments:

You may build other setups with different types of defects. Be aware that, within a band gap, the propagation of a wave is suppressed strongly by reflection at the lattice. If the defects are too far from each other, or from speaker and microphone, they cannot be observed. You may try using shorter setups that have a small number of unit cells. In this case, it is easier to observe all defect-states with sufficient amplitude.