From equation to creation: using the Schrödinger equation in an artistic context

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Abstract

In this paper the possibilities of using the Schrödinger equation in an artistic context are discussed. Firstly, the mathematics behind the equation is introduced and is given its corresponding physical meaning. Secondly, the possibilities for using the data from the equation are explored for generating images and visuals, for mapping the data to sound parameters and to control different sound and visual processes in time.

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1. Introduction

In this paper I will discuss the solution of the Schrödinger equation for hydrogen and its possible use in an artistic context rather than purely scientific. My goal in the first part of this paper is to explain what all the individual terms and components of the equation represent from a physical perspective. I'll assume that the reader has some mathematical and physical background and will give references for further reading if necessary. In the second part I will discuss some of the possibilities of using the Schrödinger equation for making visuals and mapping it to musical parameters.

2. Introduction to quantum mechanics

What is quantum mechanics and why is it so different from classical physics? Both quantum and classical mechanics give a way to describe how a physical system evolves over time. However, in classical physics you go about the fact that as long as you know the initial state of a system, then generally speaking, you can predict exactly the outcome at a later time (Feynman, 1964, volume 1: 11-1 – 11-10). This line of reasoning works fairly well for phenomena on a macroscopic level and thus with our experience in everyday life, but it turns out that on a sub-atomic level, things behave in a way completely different from this. Fundamental to this difference is the wave-particle duality of all matter and radiation and the fact that in the case where the classical approach predicts certainties, you can only predict the probability of a possible outcome in quantum mechanics.
Another key aspect that is tightly related to the above and completely in disagreement with classical mechanics is called the *Heisenberg uncertainty principle*. This addresses the fact that it turns out to be impossible to measure the momentum and the position of a particle at the same time (Feynman, 1964, volume 3: 1-11). For everyday life however, classical physics gives a good enough approximation of reality[1].

Quantum mechanics can seem like a very unreal and strange thing. The fact is that even physicists working in the field of quantum mechanics can't explain why the microscopic world behaves the way it does. The majority just accepts this fact and rather is concentrating on an accurate description of the underlying mathematical framework. To gain a little more insight in the strange behavior of

[1] The range over which quantum effects dominate over classical mechanics is incredibly small, typically the size of atoms (roughly 10^{-8}cm) or smaller.

matter on a microscopic level, you can consider the famous double-slit experiment. This also addresses the wave-particle duality of matter and radiation in an intuitive manner (Feynman, 1964, volume 3: 1-1 – 1-9).

3. The Schrödinger Equation

Before presenting the mathematics behind the Schrödinger equation, let's first state what it actually represents. The Schrödinger equation (Schrödinger, 1926) describes how the quantum state of a physical system changes over time. In the standard interpretation of quantum mechanics, the quantum state, also called a wave function or state vector, is the most complete description that can be given of a physical system[2]. This wave function is a complex valued function of only a few variables. If the wave function is normalized[3], it is possible to *absolute square* the result to obtain the probability density. This real valued function then determines the probability of finding a particle at a particular place and at a particular time. We will discuss the general form of the equation first before we consider the specific solution for a hydrogen atom.

The non-relativistic Schrödinger equation for a single particle in a scalar potential is given by the differential equation:

$$\mathrm{i}\hbar\frac{\partial}{\partial \mathrm{t}}\boldsymbol{\Psi}(\boldsymbol{r},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})\right)\boldsymbol{\Psi}(\boldsymbol{r},t)$$

Recall from classical physics that the kinetic energy of a particle is given by the relation:

$$E_k = \frac{p^2}{2m}$$

where p^2 stands for the momentum squared. If we set $V(\boldsymbol{r}) = 0$ for a moment and then compare the two equations above, we see that they are quite similar. If we let $E_k \to \mathrm{i}\hbar\frac{\partial}{\partial t}$ and $\mathbf{p} \to \frac{\hbar}{\mathrm{i}}\nabla$ where $\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)$, we can represent the classical variables for the energy and the momentum as differential operators which act on the wave function[4]. Now if the momentum squared is expressed in terms of the operator $\mathbf{p}^2 = \nabla^2$, we can write[5]:

$$-\hbar^2\nabla^2 = \left(\frac{\hbar}{\mathrm{i}}\right)^2\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$

The additional term $V(\boldsymbol{r})$ represents the potential energy of the atom which varies with position. Furthermore, let us emphasize that $V(\boldsymbol{r})$ does not depend on time explicitly, because we deal with a so-called conservative system. Finally, $\boldsymbol{\Psi}(\boldsymbol{r},t)$ is the wave function of the particle, which is the

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[2] The term "state" is rather abstract in the context of quantum theory. The reader who seeks a better explanation at this point could consider (Feynman, 1964, volume 3), (Messiah, 1961, volume 1: 294-296).

[3] The wave function is said to be normalized if the integral taken over some interval in which the particle should exist is equal to one. To be able to talk about a certain probability it is convenient if the total probability adds up to one.

[4] Readers which have difficulty in understanding the concept of differential operators, see (Feynman, 1964, Volume 2: Chapter 2).

[5] In some cases you will see Δ instead of ∇^2. This is just a matter of notation; in the end they mean the same thing.

amplitude for the particle to have a given position $\boldsymbol{r}$ at any given time[6] t. Observe that the Schrödinger equation is a first order differential equation *with respect to time* in accord with the postulate that the dynamical state of the physical system is entirely determined once $\boldsymbol{\Psi}$ is given (Messiah, 1961, volume 1: 61).

Next, let's discuss how the Schrödinger equation can be used to describe a simple system of two bodies with a Coulomb[7] interaction: the hydrogen atom. A hydrogen atom consists of a single negatively charged electron 'orbiting'[8] a nucleus made up from a positively charged proton of much larger mass. The potential energy of the electron in the electrostatic field of the proton is:

$$V = -\frac{\boldsymbol{e^2}}{r}$$

More precisely, $\boldsymbol{e^2} = \frac{q_e^2}{4\pi\epsilon_0}$, where q_e^2 is the charge of the particles and $4\pi\epsilon_0$ is a constant, and r is the distance from the location of the electron to the nucleus. If we let E be the energy of the electron-proton system then the wave function is a solution of the time-independent Schrödinger equation:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r}\right]\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

Since the potential energy term only depends on the radius, it is more convenient to solve the equation in terms of spherical coordinates (r, θ, φ) rather than rectangular coordinates. After some algebraic manipulations and the procedure of *separating of variables* (Messiah, 1961, volume 1: 343-368), we can write the solutions as a product of three separate terms:

$$\psi(r, \theta, \varphi) = R(r)\Theta(\theta)\Phi(\varphi)$$

where $R(r)$ is the radial part and the product of $\Theta(\theta)$ and $\Phi(\varphi)$ denotes the angular part in the form of *spherical harmonics* (Messiah, 1961, volume 1: 348-349). Furthermore, it turns out that the solution depends on a set of *quantum numbers*. These numbers describe values of conserved quantities in the dynamics of the quantum system. In the specific case of the hydrogen atom there are three:

- n which describes the total energy of the electron, called the principal quantum number, and takes on positive integer values $n = 1, 2$ ...
- l which is related to the angular momentum, called the azimuthal quantum number, and takes on positive integer values $0 \leq l \leq n - 1$.
- m which is the projection of the angular momentum along a specified axis, called the magnetic quantum number, and takes on integer values $-l \leq m \leq l$.

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[6] $\boldsymbol{\Psi}(\boldsymbol{r}, t)$ can also be viewed as a superposition of monochromatic plane waves: $\mathrm{e}^{\mathrm{i}(\mathbf{p}\cdot\mathbf{r}-Et)/\hbar}$, where $\frac{\mathbf{p}}{\hbar} = \mathbf{k}$ and $\frac{E}{\hbar} = \omega$, thus alternatively, $\mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\mathbf{r}-\omega t)}$ represents a vibration of wavelength $\lambda = 2\pi/k$ travelling in the direction of its wave vector $\mathbf{k}$ with constant velocity.

[7] See for a description of Coulomb's law (Feynman, 1964, volume 2: 4-2).

[8] We can't speak of an orbit in an absolute sense since we can only *predict* a possible position of the electron relative to the nucleus inside the atom.

The r dependent part $R(r)$ is defined by a set of functions called the *generalized Laguerre polynomials* and take the form:

$$R_{nl}(r) = A_{nl} e^{-\frac{\rho}{2}} \rho^l L_{n-l-1}^{2l+1}(\rho)$$

where A_{nl} is a normalization constant[9], $\rho = \frac{2r}{na_0}$ (a_0 is the Bohr radius) and $L_{n-l-1}^{2l+1}(\rho)$ are the *generalized Laguerre polynomials* of degree $n-l-1$ and order $2l+1$.
The angular part can be written as a product of *trigonometric functions* and a set of functions called the *associated Legendre functions*:

$$Y_l^m(\theta, \varphi) = N_l P_l^m(\cos\theta) e^{im\varphi}$$

where Y_l^m is a *spherical harmonic* of degree l and order m, N_l is a normalization constant[10], P_l^m is an *associated Legendre function* of degree l and order m, and θ and φ represent colatitude and longitude respectively.
Summarizing, we now have in our disposal the solution of the Schrödinger equation for a hydrogen atom. By choosing specific values for the three *quantum numbers* n, l and m, we can simulate the different quantum states of the atom. In the next section we will look at different ways of using this information.

4. Using the Schrödinger equation

4.1 And now…

At this point it might happen that the reader of this article would be asking him/herself; why bother with all of this very complicated and highly abstract material? Let's take a step back and consider the following:
Along with the more technical approaches to digital audio and physical sound, there is a rich history of composers who incorporated some mathematical or physical model into their work, either purely as a source of inspiration, but just as well as to play an active role in the composition process itself[11].
Also in the field of computer music, mathematics plays an active and important role. Obvious examples are for instance probability and chaos theory and fractals and the role these play in mapping data from equations to musical parameters. Even more obvious is the relevance of physics in animation and computer generated graphics. To make something look realistic, in the end you could not do without the laws of physics. As a concrete example consider realistic shading or the simulation of natural looking movement.

Is it possible to do the same with the Schrödinger equation? In other words, could we use the information obtained from this equation in some creative way?
In (Fischman, 2003) the author describes a way of using the Schrodinger equation in the generation of granular clouds. The clouds are derived from statistical distributions obtained from the equation. In the coming sections I will discuss some further possibilities of using the information from the equation in the generation of sounds and images and to control the evolution of them in time.

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[9] There are several different normalization constants in use. I've used: $A_{nl} = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3}}$

[10] Again, several different normalization constants are in use. In physics the constant is generally defined as: $N_l = \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}$

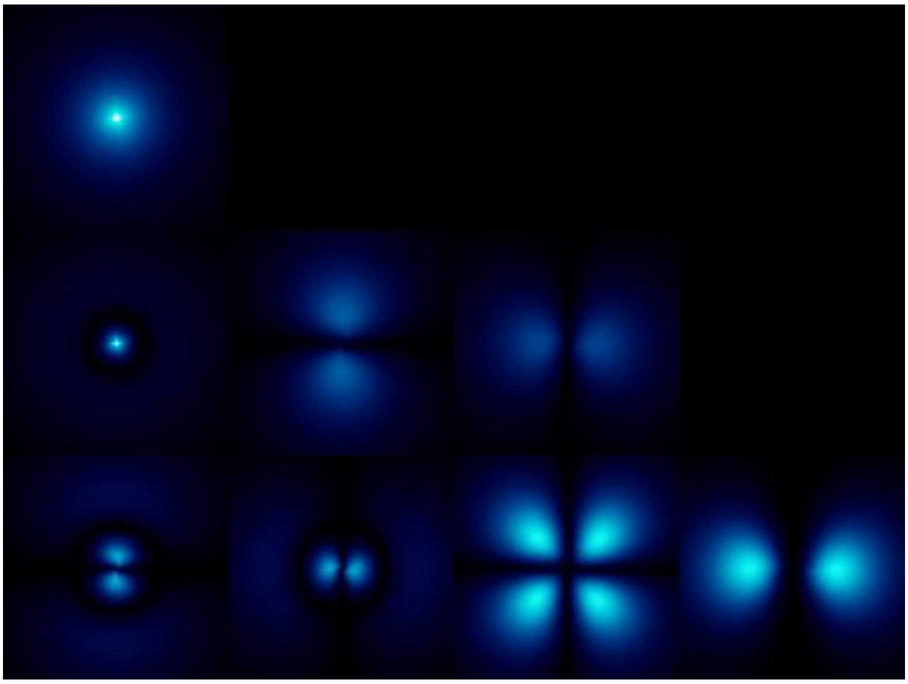
[11] The contemporary work of Iannis Xenakis is probably the best example of this.

4.2 Visualizing the probability density plots

As mentioned before, if we take the *absolute square* of the Schrödinger equation it gives us the probability density of finding a particle at a particular place in space. If we use software to do all the calculations we can generate a high resolution data stream representing this probability density. After that we are free to do with this data what we want.

The most obvious thing to do, and probably the most useful from a scientific point of view, is to visualize the data from the equation in some way or other. You could for instance map the data from the equation to color and plot the results in the form of high resolution images (see figure 1). These images could then serve as a base for making a visual composition in time. I have found that even with a minimum amount of processing you could obtain very interesting results. By rotation, zooming, horizontal and vertical stretching and translation of the images, a wide variety of interesting effects can be obtained, while keeping true to the original images. Another thing that usually works well is to use feedback with previous rotated and stretched frames.

Figure 1. Mapping the data from the Schrödinger equation to color: n ranges from 1 to 3 per row, l ranges from 0 to n – 1 per column and m ranges from 0 to l per column. Images made in Processing (http://www.processing.org).

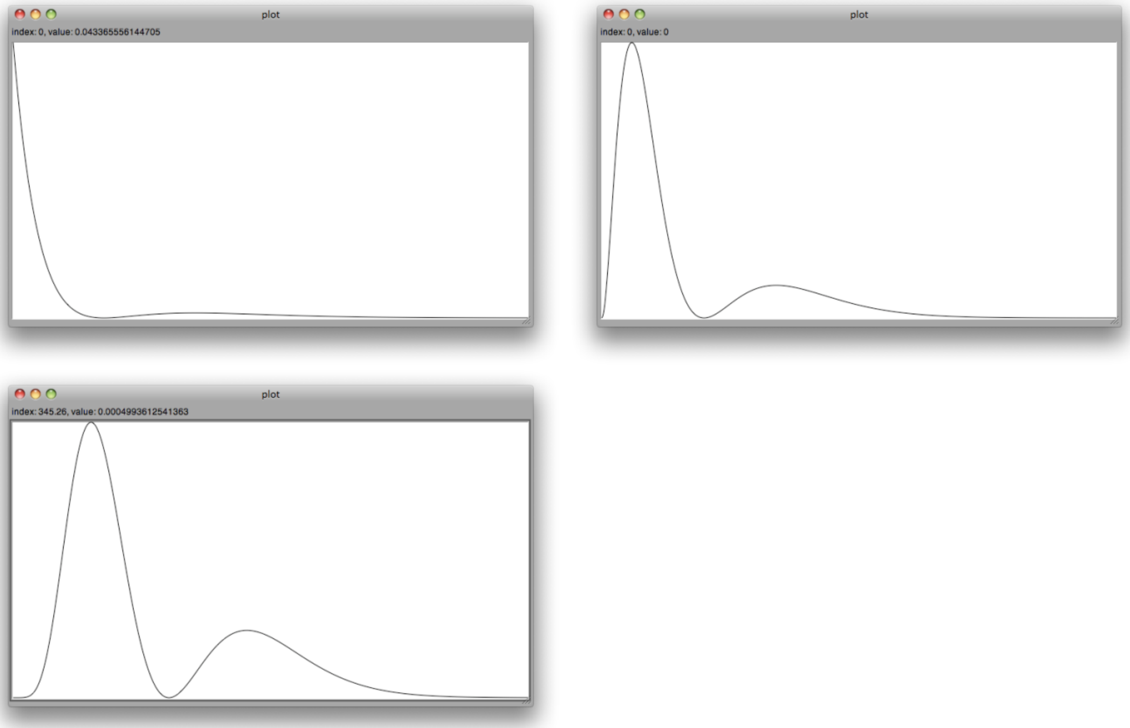


The next step would be to find a suitable way of controlling the discussed parameters in time. There are several options for this. Of course this could be done totally at random, but this will almost for sure not give the most interesting results. Something that could work a lot better is to use the data from the Schrödinger equation again. So we not only visualize the information from the equation, but we also use the same equation to control the processing of these images. Recall that the Schrödinger equation is a differential equation, which means that the solutions are all smooth, continuous curves[12]. If we then use these curves for controlling the rotation of an image for instance, this will happen in a smooth, natural way. Furthermore, because the solutions to the equation are practically infinite, we basically have an unlimited amount of curves to choose from (see figure 2). Another option would be to use data obtained from audio analysis to control the parameters for the image processing. This would add a whole new dimension to the total experience. Not only is there something to listen to, but now we have the opportunity to create a deeper relation between what the observer sees and hears.

[12] This is of course also the reason that the original images look so smooth.

The two options discussed above could of course be used in conjunction as well. There is no reason to exclusively use one or the other. Also, I discussed controlling the parameters of the visuals by means of audio analysis, but there is no reason this wouldn't work the other way around: analyzing the visuals and using this data to control certain sound processes. In most cases, analyzing the visuals probably isn't even necessary; we can just use the Schrödinger equation for this, in much the same way as we did for the visuals. This will be the topic of the next section.

Figure 2. Some curves obtained from the Schrödinger equation. From left to right: n = 2, l = 0, m = 0, 0 ≤ r ≤ 6, n = 3, l = 1, m = 1, 0 ≤ r ≤ 16 and n = 5, l = 3, m = 2, 0 ≤ r ≤ 35. Images made in Supercollider (http://supercollider.sourceforge.net).



4.3 From equation to music

In a musical context, we could use the data from the Schrödinger equation to control sound parameters in practically the same way as we did for the images. Think of the amplitude of a sound, cutoff frequency of a filter or a modulation index but to name a few. Most uses are applicable at the micro, mesa as well as the macro level. In the specific case of *granular synthesis* for instance, the curves can be used as a window for an individual grain, but just as well as an amplitude envelope for a granular cloud consisting of hundreds of grains. Another idea would be to use the data in an *additive synthesis* context, by using a curve obtained from the equation to control the frequency, amplitude and/or spatialization of a sound produced by an oscillator. By inter mixing a desired amount of oscillators in this way, a more complex and evolving sound can be generated. I did not choose the two examples of *granular* and *additive* synthesis totally at random. Besides the fact that generally a lot of parameters can be controlled, by their own nature, they also address the most fundamental and remarkable fact about quantum mechanics: the wave-particle duality of all matter and radiation.

In addition to these more or less obvious examples we could also think of more elaborate uses. Think about using all the different curves obtainable from the equation in the context of a probability weighting function. The weighted random numbers generated in this way could then be used to determine basically every parameter imaginable of a sound, like duration, amplitude, density etcetera. Incidentally, in doing so you would keep true to the original use of the Schrödinger equation as well, namely stating a certain probability.

Another possibility is to use a curve obtained from the equation as a transfer function for a lookup table. Because the Schrödinger equation is a differential equation and thus the solutions are all smooth, continuous curves, it can, after some modifications, be used in much the same way as Chebyshev polynomials to create harmonic distortion (Moore, 1990: 333 – 337).

5. Conclusions and future developments

One thing that remains to be discussed is if the use of the Schrödinger equation for generating and ordering sounds and images in time gives aesthetically pleasing results. This is for a large part a very subjective thing and it is a question that could be asked for experimental algorithmic composition methods in general. This goes beyond the scope of this article however. The only thing I would like to mention is that the results obtained are very interesting to say the least. With experimenting in this way, you can obtain results that would be a lot harder or even impossible to achieve if worked in a more conventional way. Therefore I think it is important to pursue the quest of what role mathematical and physical systems can play in the process of making a piece of art and/or software.

Another interesting effect of working with experimental algorithms is that the composer now has the possibility to diverge from the traditional way of composing. For me, the ultimate goal would be to let the algorithm decide as much as possible to the point that the composer its only task is to select an appropriate algorithm and to program the necessary software in which the algorithm can function according to the wishes of the composer. In this way the computer can generate an enormous amount of material and afterwards the composer makes a selection based on what he thinks has musical potential.

To conclude on a more philosophical note: the very mathematical and physical foundations on which our universe seems to be built are of such elegance and beauty that it may be considered only right to incorporate them in our everyday life and work as much as possible. For me personally, trying to integrate mathematical and physical models with my interests in software development, sound art and generative art is of the utmost importance. Not only out of pure interest and respect for the laws of nature, but because I think they can contribute to a work of art in their own specific way and there is still a lot to be discovered.

6. References

[1] Feynman R. P., R. B. Leighton, and M. Sands. 1971 *The Complete Feynman Lectures on Physics*. Massachusetts: Addison-Wesley.

[2] Fischman, R. 2003 "Clouds, Pyramids, and Diamonds: Applying Schrödinger's Equation to Granular Synthesis and Compositional Structure." *Computer Music Journal* 27(2): 47-96.

[3] Messiah, A. 1961 *Quantum Mechanics, Volume I*. Amsterdam: North-Holland Publishing.

[4] Moore, F. R. 1990 *Elements of Computer Music*. Upper Saddle River: Prentice-Hall.

[5] Roads, C. *Microsound*. Massachusetts: The MIT Press.

[6] Schiff, L.I. 1955 *Quantum Mechanics*. New York: McGraw-Hill.

[7] Schrödinger, E. 1926 "An Undulatory Theory of the Mechanics of Atoms and Molecules" *The Physical Review* 28(6): 1049-1070.

[8] Suurmond, P. (2002) *13 Studies in Nanotonality,* http://www.kmt.hku.nl/~pieter/CC/nano13.html, March 9, 2009.

[9] Tang, C.L. 2005. *Fundamentals of Quantum Mechanic: For Solid State Electronics and Optics*. Cambridge: Cambridge University Press .

[10] Teschl, G. (2009) *Mathematical Methods in Quantum Mechanics*, http://www.mat.univie.ac.at/~gerald/, March 3, 2009.

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