
Schrodinger Equation

Interpretation and Time-Dependence

This is our twenty-fourth notebook. In this notebook, we will build on the intuition for the solutions found in the previous notebook. We will interpret and “normalize” the solutions. These are known as stationary solutions. Then we will reintroduce time, see that energy closely relates to time-dependence, and finally combine solutions with different energies and different time-dependencies to get non-stationary (moving) solutions of Schrodinger’s equation.

Schrodinger’s Harmonic Oscillator Solution

In fact, the problem we were studying in the previous notebook, while hard, was solved exactly by Schrodinger in 1926. Here is the beginning of his paper (the whole thing is about 30 short pages):

1926

Abh. 18

ANNALEN DER PHYSIK VIERTE FOLGE. BAND 81

1. *Quantisierung als Eigenwertproblem;* *von E. Schrödinger*

(Vierte Mitteilung¹⁾)

Inhaltsübersicht: § 1. Elimination des Energieparameters aus der Schwingungsgleichung. Die eigentliche Wellengleichung. Nichtkonservative Systeme. — § 2. Ausdehnung der Störungstheorie auf Störungen, welche explizite die Zeit enthalten. Dispersionstheorie. — § 3. Ergänzungen zu § 2: Angeregte Atome, entartete Systeme, Streckenspektrum. — § 4. Erörterung des Resonanzfalles. — § 5. Verallgemeinerung für eine beliebige Störung. — § 6. Relativistisch-magnetische Verallgemeinerung der Grundgleichungen. — § 7. Über die physikalische Bedeutung des Feldskalars.

§ 1. Elimination des Energieparameters aus der Schwingungsgleichung. Die eigentliche Wellengleichung. Nichtkonservative Systeme

Die Wellengleichung (18) bzw. (18') von S. 510 der zweiten Mitteilung

$$(1) \quad \Delta \psi - \frac{2(E - V)}{E^2} \frac{\partial^2 \psi}{\partial t^2} = 0$$

bzw.

$$(1') \quad \Delta \psi + \frac{8\pi^2}{h^2} (E - V) \psi = 0,$$

Let us note, for completeness, that Heisenberg independently solved the harmonic oscillator, but Heisenberg’s approach is unrecognizably different than what we are doing, so I won’t have anything more to say about it.

Exact Energy Levels

One of the things that comes out of an exact solution is the exact energy levels. They are:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

First we should compare that with the values we got by fiddling with energy in the previous notebook.

$$\text{In}[*]:= \text{energy}[n_]:= n + \frac{1}{2}$$

Allowing for “experimental” error, did you get something close to $\frac{1}{2}$, $\frac{3}{2}$, $\frac{5}{2}$, $\frac{7}{2}$, and $\frac{9}{2}$?

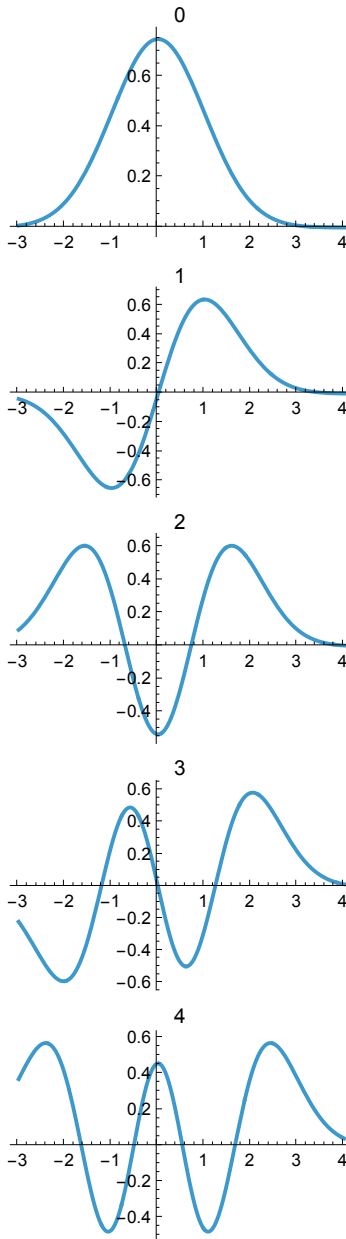
Exact Solutions (Wave Functions)

The other thing that comes out of an exact solution is the exact wave functions, but rather than attempt to give you some kind of general formula for $\psi_n(x)$ that is valid for all n , I’ll just define the first five (with $n = 0, 1, 2, 3$, and 4):

$$\begin{aligned} \text{In}[*]:= \text{psi}[x_, 0] &:= \frac{1}{\text{Pi}^{1/4}} \text{Exp}[-x^2/2]; \\ \text{psi}[x_, 1] &:= \frac{1}{\text{Pi}^{1/4}} \sqrt{2} \, x \, \text{Exp}[-x^2/2]; \\ \text{psi}[x_, 2] &:= \frac{1}{\text{Pi}^{1/4}} \frac{1}{\sqrt{2}} (2x^2 - 1) \, \text{Exp}[-x^2/2]; \\ \text{psi}[x_, 3] &:= \frac{1}{\text{Pi}^{1/4}} \frac{1}{\sqrt{3}} (2x^3 - 3x) \, \text{Exp}[-x^2/2]; \\ \text{psi}[x_, 4] &:= \frac{1}{\text{Pi}^{1/4}} \frac{1}{\sqrt{384}} (16x^4 - 48x^2 + 12) \, \text{Exp}[-x^2/2]; \end{aligned}$$

Let’s plot those five:

```
In[ ]:= Table[Plot[psi[x, n], {x, -3, 4}, PlotLabel -> n], {n, 0, 4}] // Column
Out[ ]:=
```



Again you could compare with your crude plots from the previous notebook.

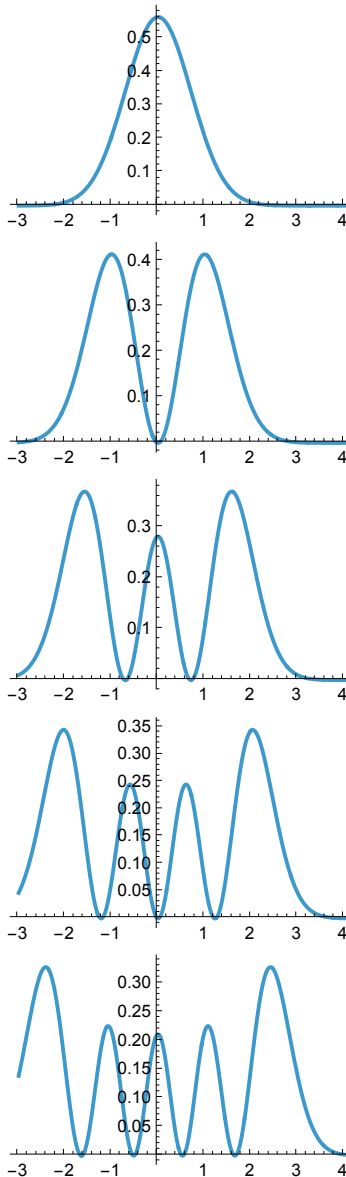
Exact Solutions — Interpretation — Normalization

The next intellectual leap that the quantum physicists of the 1920s made is that the wave function is itself unobservable! Furthermore they allowed the value of the wave function at each point x (or at each point x at each time t) to be a complex number!! Complex numbers are numbers that can have both real and imaginary parts. It's almost like these guys were tripping. I cannot fathom how they came up with such crazy stuff.

Anyway, if you square the wave function (thereby losing some information), what comes out of that operation is the thing that is observable. The observable is interpreted as the probability of finding the particle at the point in question. The “squaring” I am talking about always yields a real number. In Mathematica we will use `Abs[]` and then square the result, because `Abs[]` has been arranged to do the right thing with complex numbers.

The wave functions I tabulated above were already real, so I could have used ordinary squaring, but let’s already start getting in the habit of using the kind of squaring you have to use when complex numbers appear. Let’s plot the squared wave functions:

```
In[ ]:= Table[Plot[Abs[psi[x, n]]^2, {x, -3, 4}], {n, 0, 4}] // Column
Out[ ]:=
```



Because the interpretation of the square of the wave function is that it is the probability for finding the particle at a position, and the probability of finding the electron somewhere must be one, then the sum

of the probability of finding it any specific place must add up to 1. You can eyeball the curves above and perhaps satisfy yourself that they each have area under the curve 1, or you can make Mathematica compute the area under each of the curves:

```
In[*]:= Table[Integrate[Abs[psi[x, n]]^2, {x, -Infinity, Infinity}], {n, 0, 4}]
Out[*]:= {1, 1, 1, 1, 1}
```

Now you finally know why $\psi'(-\text{longWays}) = 0.1$ was arbitrary. We were just going to multiply by a constant so that the total probability came out to 1. That is precisely the reason for all the messy constants like $\frac{1}{\sqrt{1/4}}$ $\frac{1}{\sqrt{384}}$ that showed up out in front of the exact wave functions. These are called “normalized” wave functions.

Quantum Superpositions

Quantum mechanics allows any superposition of wave functions to be a wave function. Let's consider an arbitrary superposition of the first five wave functions. The most general superposition, now including the time dependence looks like this:

```
In[*]:= timeDependentPsi[x_, t_] :=
  Expand[Sum[c[n] * psi[x, n] Exp[-Sqrt[-1] energy[n] t], {n, 0, 4}]]
timeDependentProbabability[x_, t_] := Abs[timeDependentPsi[x, t]]^2
timeDependentProbabability[x, t] // TraditionalForm
```

Out[*]//TraditionalForm=

$$\left| \frac{\frac{\sqrt{2}}{3} e^{-\frac{x^2}{2} - \frac{9it}{2}} c(4) x^4}{\sqrt[4]{\pi}} + \frac{2 e^{-\frac{x^2}{2} - \frac{7it}{2}} c(3) x^3}{\sqrt{3} \sqrt[4]{\pi}} + \frac{\sqrt{2} e^{-\frac{x^2}{2} - \frac{5it}{2}} c(2) x^2}{\sqrt[4]{\pi}} - \frac{\sqrt{6} e^{-\frac{x^2}{2} - \frac{9it}{2}} c(4) x^2}{\sqrt[4]{\pi}} + \right.$$

$$\left. \frac{\sqrt{2} e^{-\frac{x^2}{2} - \frac{3it}{2}} c(1) x}{\sqrt[4]{\pi}} - \frac{\sqrt{3} e^{-\frac{x^2}{2} - \frac{7it}{2}} c(3) x}{\sqrt[4]{\pi}} + \frac{e^{-\frac{x^2}{2} - \frac{it}{2}} c(0)}{\sqrt[4]{\pi}} - \frac{e^{-\frac{x^2}{2} - \frac{5it}{2}} c(2)}{\sqrt{2} \sqrt[4]{\pi}} + \frac{\sqrt{\frac{3}{2}} e^{-\frac{x^2}{2} - \frac{9it}{2}} c(4)}{2 \sqrt[4]{\pi}} \right|^2$$

Are you not glad we have Mathematica to do this algebra for us?

Animating Time Dependence

So that the total probability in the superposition of finding the electron somewhere is still 1, we must have:

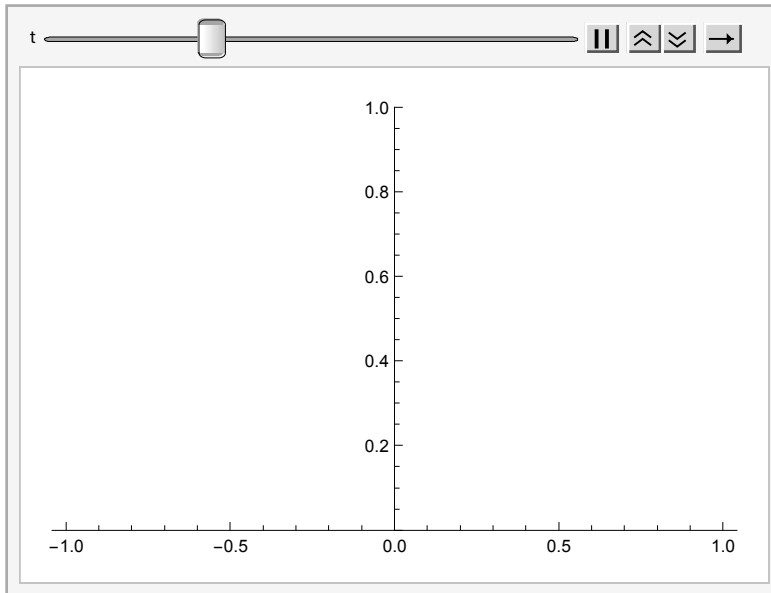
$$\text{Abs}[c[0]]^2 + \text{Abs}[c[1]]^2 + \text{Abs}[c[2]]^2 + \text{Abs}[c[3]]^2 + \text{Abs}[c[4]]^2 = 1$$

A Trivial Cross-Check

If we take a pure state, one that only has $c[2]=1$ for example, and all the rest 0, we should get back a stationary probability density function. Let's do that case:

```
In[*]:= Animate[Plot[
  timeDependentProbabability[x, t] /. {c[0] → 0, c[1] → 0, c[2] → 1, c[3] → 0, c[4] → 0},
  {x, -4, 4}, PlotRange → {All, {0, 1}}, {t, 0, 2 Pi}]
```

Out[*]=



A Non-Trivial Superposition

What solution of $\text{Abs}[c[0]]^2 + \text{Abs}[c[1]]^2 + \text{Abs}[c[2]]^2 + \text{Abs}[c[3]]^2 + \text{Abs}[c[4]]^2 = 1$ can you come up with that has $c[2]=c[3]=c[4]=0$ and $c[1]=c[2]$? Copy-and-paste the essential part out of the Animate[] above, make the necessary changes, and put it into the animate below:

```
In[ ]:= Animate[Graphics[Disk[]], {t, 0, 2 Pi}]
```

Out[]=

