Schrodinger Equation — Two and Three Dimensions

Particle Confined to a Disk, the Hydrogen Atom

Completed and Analyzed in class, May 2, 2025

This is our twenty-fifth and last notebook. In the twenty-fourth notebook, we interpreted the solutions of Schrodinger's Equation, and we added combinations of solutions with different energies together to create time-dependent solutions.

Classical Circular Drumhead — Theory Recap

To do the circular drumhead back in the fifteenth notebook, we introduced polar coordinates. The second derivative with respect to both directions takes a distinctly different form in polar coordinates. See https://www.math.ucdavis.edu/~saito/courses/21C.w11/polar-lap.pdf if you want a derivation, and I can tell you that you almost certainly don't. Just believe the bottom line that our partial differential equation in the interior of the drumhead becomes

$$\frac{\partial^2 z}{\partial t^2} = v_0{}^2\left(\frac{\partial^2 z}{\partial r^2} + \frac{1}{r}\,\frac{\partial^2 z}{\partial r^2} + \frac{1}{r^2}\,\frac{\partial^2 z}{\partial \theta^2}\right)$$

Quantum Particle Confined to a Disk

$$\frac{\partial^2 z}{\partial t^2} = v_0{}^2\left(\frac{\partial^2 z}{\partial r^2} + \frac{1}{r}\,\frac{\partial^2 z}{\partial r^2} + \frac{1}{r^2}\,\frac{\partial^2 z}{\partial \theta^2}\right)$$

```
Module[{v0 = 1}, {Derivative[2, 0, 0][z][t, r, θ] ==
    v0^2 (Derivative[0, 2, 0][z][t, r, θ] + 1/r Derivative[0, 1, 0][z][t, r, θ] +
       1/r^2 Derivative[0, 0, 2][z][t, r, θ])}] // TraditionalForm
```

Yet More Partial Derivatives

Now that we have polar coordinates, we will have things like this:

```
In[ ]:= 1/r^2 Derivative[0, 0, 2][z][t, r, θ] // TraditionalForm
Out[ ]//TraditionalForm=
```

$$\frac{z^{(0,0,2)}(t, r, \theta)}{r^2}$$

The Circular Drumhead Differential Equation

Recopying what was above, you can give Mathematica this differential equation:

$$\frac{\partial^2 z}{\partial t^2} = v_0{}^2\left(\frac{\partial^2 z}{\partial r^2} + \frac{1}{r}\,\frac{\partial^2 z}{\partial r^2} + \frac{1}{r^2}\,\frac{\partial^2 z}{\partial \theta^2}\right)$$

In[∘]:=
```
Module[{v0 = 1}, {Derivative[2, 0, 0][z][t, r, θ] ==
    v0^2 (Derivative[0, 2, 0][z][t, r, θ] + 1/r Derivative[0, 1, 0][z][t, r, θ] +
       1/r^2 Derivative[0, 0, 2][z][t, r, θ])}] // TraditionalForm
```
Out[∘]//TraditionalForm=

$$\left\{z^{(2,0,0)}(t, r, \theta) = \frac{z^{(0,0,2)}(t, r, \theta)}{r^2} + \frac{z^{(0,1,0)}(t, r, \theta)}{r} + z^{(0,2,0)}(t, r, \theta)\right\}$$

First Massive Simplification — Assumption of Circular Symmetry

I'll say, that this is pretty advanced stuff that I am getting you into, and I want to back off a bit just to push it through to a conclusion. The massive simplification will be to simplify our function of z to not depend on θ. We are only going to be looking at circularly symmetric solutions of the drumhead equation. This means when we get to the point of striking the drumhead with a mallet, we are going to have to strike it dead center, and with a mallet whose head is circularly symmetric.

With this first massive simplification the equation becomes:

Recopying what was above, you can give Mathematica this differential equation:

$$\frac{\partial^2 z}{\partial t^2} = v_0{}^2\left(\frac{\partial^2 z}{\partial r^2} + \frac{1}{r}\,\frac{\partial z}{\partial r}\right)$$

In[∘]:=
```
Module[{v0 = 1}, {Derivative[2, 0][z][t, r] ==
    v0^2 (Derivative[0, 2][z][t, r] + 1/r Derivative[0, 1][z][t, r])}] // TraditionalForm
```
Out[∘]//TraditionalForm=

$$\left\{z^{(2,0)}(t, r) = \frac{z^{(0,1)}(t, r)}{r} + z^{(0,2)}(t, r)\right\}$$

Second Simplification — An Insight

One of the terms in our equation seems to blow up at $r = 0$. Perhaps this blowing up represents infinite acceleration at the center of the drum!? NO!! That is unphysical. It must be that that the first derivative on the right hand side and the second derivative on the right hand side conspire, when added together, to not blow up. Perhaps if we explicitly put in a power of r into the solution, we can discover what power of r yields an acceptable combination of first and second derivatives.

So the insight leads to the ansatz

$z(t, r) = r^{\mu}\,\rho(t, r)$

Putting this ansatz into the differential equation, we get the new differential equation,

$$r^\mu \frac{\partial^2\rho}{\partial t^2} = v_0{}^2\left(\mu(\mu-1)\, r^{\mu-2}\, \rho + 2\,\mu\, r^{\mu-1} \frac{\partial\rho}{\partial r} + r^\mu \frac{\partial^2\rho}{\partial r^2} + \frac{1}{r}\,\mu\, r^{\mu-1}\, \rho + \frac{1}{r}\, r^\mu \frac{\partial\rho}{\partial r}\right)$$

Divide through by r^μ and combine like terms

$$\frac{\partial^2\rho}{\partial t^2} = v_0{}^2\left(\mu^2 \frac{1}{r^2}\, \rho + (2\,\mu\, + 1)\, \frac{1}{r} \frac{\partial\rho}{\partial r} + \frac{\partial^2\rho}{\partial r^2}\right)$$

With $\mu = -\frac{1}{2}$ we can make the first derivative term go away. Then multiply through by r^2 and we have

$$r^2 \frac{\partial^2\rho}{\partial t^2} = v_0{}^2\left(\frac{1}{4}\,\rho + r^2 \frac{\partial^2\rho}{\partial r^2}\right)$$

Adding the Boundary Conditions

Let’s recap before adding the boundary conditions. We have transformed our differential equation by making the substitution

$$z(t, r) = \frac{1}{\sqrt{r}}\, \rho(t, r)$$

At the boundary of the drumhead, we need $z(t, r)$ (or $\rho(t, r)$) to be zero. So that z does not blow up at $r = 0$ we also need $\rho(t, r)$ to be zero at $r = 0$.

In[ ]:=
```
drumheadRadius = 1;

Module[{v0 = 1},
  {Derivative[2, 0, 0][z][t, r, θ] == v0^2 (Derivative[0, 2, 0][z][t, r, θ] +
       1/r Derivative[0, 1, 0][z][t, r, θ] + 1/r^2 Derivative[0, 0, 2][z][t, r, θ]),
   z[t, drumheadRadius, θ] == 0, z[t, r, -Pi] == z[t, r, Pi]}] // TraditionalForm
```

Out[ ]//TraditionalForm=

$$\left\{z^{(2,0,0)}(t,r,\theta) = \frac{z^{(0,0,2)}(t,r,\theta)}{r^2} + \frac{z^{(0,1,0)}(t,r,\theta)}{r} + z^{(0,2,0)}(t,r,\theta),\ z(t,1,\theta) = 0,\ z(t,r,-\pi) = z(t,r,\pi)\right\}$$

Adding the Initial Conditions for The Drumhead

We are also missing any specification of the initial motion of the drumhead. It isn’t just going to start vibrating by itself. Here is an initial displacement function:

In[ ]:=
```
amplitude = 1;
radialMode = 2;
angularMode = 1;

f[r_, θ_] := amplitude Sin[θ] r^2 (r - drumheadRadius)
```

As you can see, we can specify a mode number in either axis. Add that to the equations and also have the initial velocity be zero:

In[ ]:=
```
Module[{v0 = 1},
  {Derivative[2, 0, 0][z][t, r, θ] == v0^2 (Derivative[0, 2, 0][z][t, r, θ] +
       1/r Derivative[0, 1, 0][z][t, r, θ] + 1/r^2 Derivative[0, 0, 2][z][t, r, θ]),
   z[t, drumheadRadius, θ] == 0, z[t, r, -Pi] == z[t, r, Pi], z[0, r, θ] == f[r, θ],
   Derivative[1, 0, 0][z][0, r, θ] == 0}] // TraditionalForm
```

Out[ ]//TraditionalForm=

$$\left\{z^{(2,0,0)}(t,r,\theta)=\frac{z^{(0,0,2)}(t,r,\theta)}{r^2}+\frac{z^{(0,1,0)}(t,r,\theta)}{r}+z^{(0,2,0)}(t,r,\theta),\right.$$
$$\left.z(t,1,\theta)=0,\ z(t,r,-\pi)=z(t,r,\pi),\ z(0,r,\theta)=(r-1)\,r^2\sin(\theta),\ z^{(1,0,0)}(0,r,\theta)=0\right\}$$

Have Mathematica Solve the Problem

In[ ]:=
```
circularDrumheadProblem = Module[{v0 = 1},
  {r^2 Derivative[2, 0, 0][z][t, r, θ] == v0^2 (r^2 Derivative[0, 2, 0][z][t, r, θ] +
       rDerivative[0, 1, 0][z][t, r, θ] + Derivative[0, 0, 2][z][t, r, θ]),
   z[t, drumheadRadius, θ] == 0, z[t, r, -Pi] == z[t, r, Pi], z[0, r, θ] == f[r, θ],
   Derivative[1, 0, 0][z][0, r, θ] == 0}]
```

Out[ ]=

$$\{r^2 z^{(2,0,0)}[t, r, \theta] == z^{(0,0,2)}[t, r, \theta] + r\, z^{(0,1,0)}[t, r, \theta] + r^2 z^{(0,2,0)}[t, r, \theta],$$
$$z[t, 1, \theta] == 0,\ z[t, r, -\pi] == z[t, r, \pi],$$
$$z[0, r, \theta] == (-1 + r)\, r^2 \mathrm{Sin}[\theta],\ z^{(1,0,0)}[0, r, \theta] == 0\}$$

In[ ]:=
```
DSolve[circularDrumheadProblem, z, {t, 0, 1}, {r, 0, drumheadRadius}, {θ, -Pi, Pi}]
```

Out[ ]=

$$\mathrm{DSolve}[\{r^2 z^{(2,0,0)}[t, r, \theta] == z^{(0,0,2)}[t, r, \theta] + r\, z^{(0,1,0)}[t, r, \theta] + r^2 z^{(0,2,0)}[t, r, \theta],$$
$$z[t, 1, \theta] == 0,\ z[t, r, -\pi] == z[t, r, \pi],\ z[0, r, \theta] == (-1 + r)\, r^2 \mathrm{Sin}[\theta],$$
$$z^{(1,0,0)}[0, r, \theta] == 0\},\ z,\ \{t, 0, 1\},\ \{r, 0, 1\},\ \{\theta, -\pi, \pi\}]$$