Schrodinger Equation — Two Dimensions

Particle Confined to a Disk

Completed and Analyzed in class, May 2, 2025

This is our twenty-fifth and next-to-last notebook. In the previous two notebooks, we introduced Schrodinger's equation, interpreted the solutions, and added combinations of solutions with different energies together to create time-dependent solutions. However, we did all that that in only one dimension. In this notebook we graduate to two dimensions.

To make graduating to two dimensions easier, I am going to do the free particle (the potential is going to be zero).

Time-Independent Schrodinger Equation in Two Dimensions

Perhaps it will not surprise you that the only new thing as we graduate to two dimensions is that instead of second derivatives with respect to *x* we now have second derivatives with respect to both *x* and *y*.

Here is the time-independent Schrodinger equation in two dimensions:

In[∘]:=
```
-ℏ^2/(2 μ) (Derivative[2, 0][ψ][x, y] + Derivative[0, 2][ψ][x, y]) +
  potential[x, y] × ψ[x, y] == energy ψ[x, y] // TraditionalForm
```

Out[∘]//TraditionalForm=

$$\text{potential}(x,y)\,\psi(x,y)-\frac{\hbar^2\left(\psi^{(0,2)}(x,y)+\psi^{(2,0)}(x,y)\right)}{2\,\mu}=\text{energy}\,\psi(x,y)$$

I changed the mass to μ in anticipation of the fact that we are going to want to use the letter *m* for something else later on. Perhaps it matters little because I am about to set $\mu = 1$.

Now let's simplify for the free particle. The potential when the particle is free (no forces) is zero. While I am at it, I will also set $\hbar = \mu = 1$:

In[∘]:=
```
Module[{ℏ = 1, μ = 1}, -ℏ^2/(2 μ) (Derivative[2, 0][ψ][x, y] + Derivative[0, 2][ψ][x, y]) ==
  energy ψ[x, y]] // TraditionalForm
```

Out[∘]//TraditionalForm=

$$\frac{1}{2}\left(-\psi^{(0,2)}(x,y)-\psi^{(2,0)}(x,y)\right)=\text{energy}\,\psi(x,y)$$

It would be easy to solve this equation in a rectangular region, but we're going to confine the particle to a disk instead. To do this, I need to bring back some stuff we used for the classical drumhead.

Classical Circular Drumhead — Essential Theory Recap

To do the circular drumhead back in the fifteenth notebook, we introduced polar coordinates. The second derivative with respect to both directions took 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 (but I can tell you that you almost certainly don't). Just remember the bottom line that the combination of second derivatives in the interior of the drumhead became:

$$\frac{\partial^2 z}{\partial x^2} + \frac{\partial^2 z}{\partial y^2} = \frac{\partial^2 z}{\partial r^2} + \frac{1}{r}\frac{\partial z}{\partial r} + \frac{1}{r^2}\frac{\partial^2 z}{\partial \phi^2}$$

Quantum Particle Confined to a Disk

Now we have enough theory to rewrite, in polar coordinates, the time-independent Schrodinger equation for a free particle confined to a disk:

```
Module[{ℏ = 1, μ = 1}, -ℏ^2/(2 μ) (Derivative[2, 0][ψ][r, ϕ] + 1/r Derivative[1, 0][ψ][r, ϕ] +
      Derivative[0, 2][ψ][r, ϕ]) == energy ψ[r, ϕ]] // TraditionalForm
```

Out[ ]//TraditionalForm=

$$\frac{1}{2}\left(-\psi^{(0,2)}(r,\theta) - \frac{\psi^{(1,0)}(r,\theta)}{r} - \psi^{(2,0)}(r,\theta)\right) = \text{energy}\ \psi(r,\theta)$$

A Great Simplification — Separation of Variables

Now we need the great trick from the twenty-first notebook, which was called "separation of variables."
We ***guess*** that $\psi(r,\phi) = R(r)\,\Phi(\phi)$.

Upon putting this guess into the differential equations, we ***discover*** that if this trick is to work, then $\Phi(\phi)$ must satisfy the ordinary differential equation:

$$\frac{d^2\Phi}{d\phi^2} = -M\,\Phi$$

If M is negative, the solutions are runaway exponentials. If M is positive, the solutions are sines and cosines. To eliminate the runaway exponentials and force $M > 0$, we write $M = m^2$ where m is some number (not to be confused with the mass, which we renamed μ).

The solutions of $\frac{d^2\Phi}{d\phi^2} = -m^2\,\Phi$ are $\Phi(\phi) = \cos m\phi$ and $\Phi(\phi) = \sin m\phi$, or any combination of those two solutions. In fact, there are imaginary combinations that are very commonly used and they are $e^{im\phi}$

Now it would make little sense to have ϕ increase by 2π and not get back the same solution. So it must be that regardless of whether we are considering $\cos m\phi$ or $\sin m\phi$ or the imaginary combinations, that m is an integer.

Now we turn our attention to $R(r)$. It must satisfy:

$$-\frac{1}{2}\left(\frac{d^2 R}{d r^2} + \frac{1}{r}\frac{dR}{d r} - \frac{m^2}{r^2} R\right) = \text{energy}\, R$$

More Simplifications

Two of the terms in our equation seem to blow up at $r = 0$. Perhaps this blowing up means that the wave function has a kink or an infinity at $r = 0$? NO! Nothing special is happening there. It must be that that the derivatives conspire, when added together, to not blow up. Let's multiply through by $-2\,r^2$ and get an equation that looks less problematic at $r = 0$:

$$r^2 \frac{d^2 R}{d r^2} + r\frac{dR}{d r} - m^2 R = -2\,r^2\,\text{energy}\, R$$

It is common to let $\epsilon = 2$ energy, and also to let $\rho = \sqrt{\epsilon}\, r$, and then the equation is:

$$\rho^2 \frac{d^2 R}{d \rho^2} + \rho\frac{dR}{d \rho} - m^2 R = -\rho^2 R$$

This appears to eliminate energy (or ϵ) from the equation completely, but the energy is hiding in the definition of ρ.

Adding the Boundary Conditions

We have a free particle, but it is only free inside the disk. At the edge of the disk, e.g., at $r = a$, the particle is prevented from escaping. So $\psi(r, \theta)$ at $r = a$ must be 0. This tells us that $R(\rho) = 0$ at $\rho = \sqrt{\epsilon}\, a$. ***This is what forces the quantization of the energy into special values!***

We have already set $\hbar = \mu = 1$, but we didn't have a spring constant, k, in this problem, so we still have the freedom to set one more dimensionful quantity to 1, and so we set the radius of the disk, $a = 1$.

```
In[ ]:= particleConfinedToADiskProblem[ϵ_, m_] := Module[{ħ = 1, μ = 1, a = 1},
  {-ħ^2/(2 μ) (ρ^2 Derivative[2][R][ρ] + ρ Derivative[1][R][ρ] + (ρ^2 - m^2) R[ρ]) == 0,
   R[Sqrt[ϵ a]] == 0}]
```

I'd like to stuff this into **DSolve** or **NDSolve** to show you that Mathematica and I are up to the challenge of solving the problem now that we have set it all up. Instead (because I am not quite up to the challenge, although I am sure Mathematica is), I am just going to quote the exact solutions.

The Exact Solutions

The exact solutions are:

$$\psi_m(\rho, \phi) = J_m(z_{m,j}\,\rho)\,e^{i m \phi}$$

If we square these, the $e^{i m \phi}$ goes away. The $z_{m,j}$ are constants chosen to make $R\left(\sqrt{\epsilon}\right) = 0$. They are "zeros of Bessel functions." The J_m are "Bessel functions of the first kind."

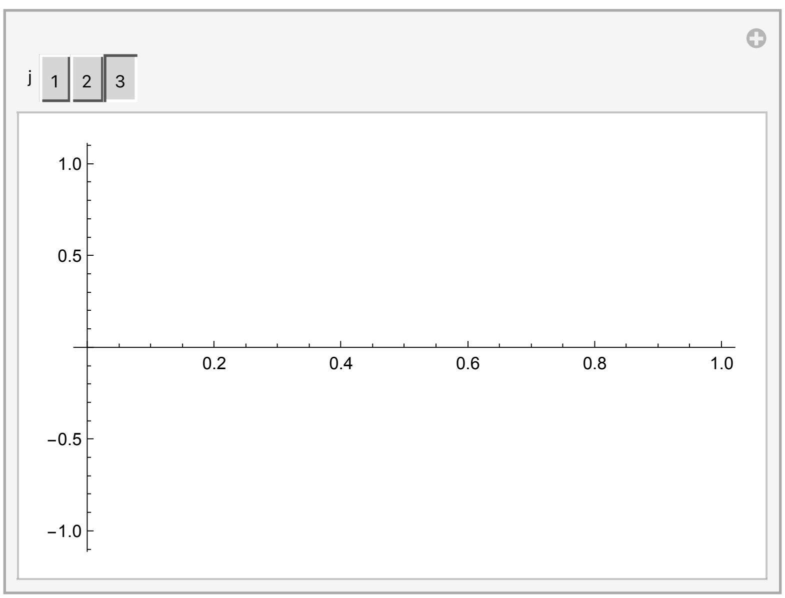
Happily for us, Mathematica knows these functions and these constants. So let's get these solutions into Mathematica:

```
In[∘]:= psiSquared[m_, j_, ρ_] := BesselJ[m, BesselJZero[m, j] ρ]^2
```

Visualizing the Exact Solutions

Finally, even though I have not done much less than I wanted to do, we can plot the exact solutions. Here are the ones with $m = 3$. The possible values of j for this value of m are $j = 1, 2, 3$.

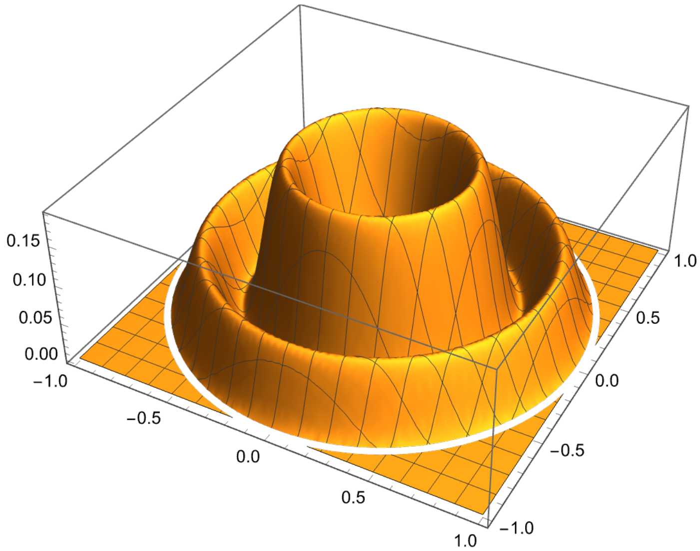
```
In[∘]:= Manipulate[Plot[psiSquared[3, j, ρ], {ρ, 0, 1}], {j, {1, 2, 3}}]
Out[∘]=
```



Also, if it helps you do visualize the probability better, we can plot the probability as a if it were a height above the disk for one of the solutions:

In[ ]:=
```
Plot3D[If[x^2 + y^2 ≥ 1, 0, psiSquared[3, 2, Sqrt[x^2 + y^2]]],
  {x, -1, 1}, {y, -1, 1}, MaxRecursion → 6]
```

Out[ ]=



Normalization

We really ought to be integrating the **psiSquared** functions and then multiplying them by a constant so that their integrals are forced to be 1. That would capture the fact that the particle must have probability 1 of being somewhere.

Time-Dependence

It would be fun to take combinations of these solutions with different energies and animate them, like we did with the harmonic oscillator. Instead, we will turn to our final topic, the Hydrogen atom.