**Derivation of Laplacian in Polar Coordinates**

Polar Coordinates

Recall the Schrödinger equation:

$$-\frac{ℏ^{2}}{2m}∇^{2}Ψ(x,y)+V\left(x,y\right)Ψ(x,y)=EΨ(x,y)$$

The Laplacian operator for two dimensional rectangular coordinates is given by:

$$∇^{2}=\frac{∂^{2}}{∂x^{2}}+\frac{∂^{2}}{∂y^{2}},$$

And when applied to a wave function $Ψ\left(x,y\right)$:

$$∇^{2}Ψ\left(x,y\right)=\frac{∂^{2}Ψ}{∂x^{2}}+\frac{∂^{2}Ψ}{∂y^{2}}.$$

Sometimes it is more suitable to describe $Ψ$ in terms of polar coordinates, i.e. $Ψ(r,θ)$. In these cases we must express the Laplacian operator in terms of polar coordinates. The following is derivation of the polar form of the Laplacian.

Recall the conversion formulae:

|  |  |
| --- | --- |
| **Polar 🡪 Rectangular** | **Rectangular 🡪 Polar** |
| $$x=rcos\left(θ\right),$$ | $$r=\sqrt{x^{2}+y^{2}}$$ |
| $$y=rsin\left(θ\right).$$ | $$θ=tan^{-1}\left(^{y}/\_{x}\right)$$ |

Below is a table of partial derivatives for $r$ and $θ$ that is useful in the derivation. The expressions are initially rendered in rectangular coordinates, and then converted to polar:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **Partial Derivatives** | **Rectangular** | **🡪** | **Polar** |
| $$r=\sqrt{x^{2}+y^{2}}$$ | $$\frac{∂r}{∂x}$$ | $$\frac{x}{\sqrt{x^{2}+y^{2}}}$$ | $$\frac{rcos\left(θ\right)}{r}$$ | $$cos\left(θ\right)$$ |
| $$\frac{∂r}{∂y}$$ | $$\frac{y}{\sqrt{x^{2}+y^{2}}}$$ | $$\frac{rsin\left(θ\right)}{r}$$ | $$sin\left(θ\right)$$ |
| $$θ=tan^{-1}\left(^{y}/\_{x}\right)$$ | $$\frac{∂θ}{∂x}$$ | $$-\frac{y}{x^{2}+y^{2}}$$ | $$-\frac{rsin\left(θ\right)}{r^{2}}$$ | $$-\frac{sin\left(θ\right)}{r}$$ |
| $$\frac{∂θ}{∂y}$$ | $$\frac{x}{x^{2}+y^{2}}$$ | $$\frac{rcos\left(θ\right)}{r^{2}}$$ | $$\frac{cos\left(θ\right)}{r}$$ |

Using classical partial derivative formulas to find ${∂Ψ}/{∂x}$:

$$\frac{∂Ψ}{∂x}=\frac{∂Ψ}{∂r}\frac{∂r}{∂x}+\frac{∂Ψ}{∂θ}\frac{∂θ}{∂x}.$$

Then substituting polar expressions for ${∂r}/{∂x}$ and ${∂θ}/{∂x}$ from the table above:

$$\frac{∂Ψ}{∂x}=cos\left(θ\right)\frac{∂Ψ}{∂r}-\frac{1}{r}\sin(\left(θ\right))\frac{∂Ψ}{∂θ}.$$

Expressing the result as an operator:

$$\frac{∂}{∂x}= cos\left(θ\right)\frac{∂}{∂r}-\frac{sin\left(θ\right)}{r}\frac{∂}{∂θ} .$$

Continue by finding an expression for ${∂^{2}Ψ}/{∂x^{2}}$:

$$\frac{∂^{2}Ψ}{∂x^{2}}=\frac{∂}{∂x}\frac{∂Ψ}{∂x}.$$

Using the results from above:

$$\frac{∂^{2}Ψ}{∂x^{2}}= \left(cos\left(θ\right)\frac{∂}{∂r}-\frac{sin\left(θ\right)}{r}\frac{∂}{∂θ}\right)\left(cos\left(θ\right)\frac{∂Ψ}{∂r}-\frac{sin\left(θ\right)}{r}\frac{∂Ψ}{∂θ}\right).$$

Expanding :

$$\frac{∂^{2}Ψ}{∂x^{2}}=cos\left(θ\right)\frac{∂}{∂r}\left(cos\left(θ\right)\frac{∂Ψ}{∂r}\right)-cos\left(θ\right)\frac{∂}{∂r}\left(\frac{sin\left(θ\right)}{r}\frac{∂Ψ}{∂θ}\right)-\frac{sin\left(θ\right)}{r}\frac{∂}{∂θ} \left(cos\left(θ\right)\frac{∂Ψ}{∂r}\right)+\frac{sin\left(θ\right)}{r}\frac{∂}{∂θ}\left(\frac{sin\left(θ\right)}{r}\frac{∂Ψ}{∂θ}\right).$$

Solving the partial derivatives (note several instances of the product rule are applied here):

$$\frac{∂^{2}Ψ}{∂x^{2}}=cos^{2}\left(θ\right)\frac{∂^{2}Ψ}{∂r^{2}}+\frac{cos\left(θ\right)sin\left(θ\right)}{r^{2}}\frac{∂Ψ}{∂θ}-\frac{cos\left(θ\right)sin\left(θ\right)}{r}\frac{∂^{2}Ψ}{∂r∂θ}+\frac{sin^{2}\left(θ\right)}{r}\frac{∂Ψ}{∂r}-\frac{cos\left(θ\right)sin\left(θ\right)}{r}\frac{∂^{2}Ψ}{∂r∂θ}+\frac{cos⁡(θ)sin\left(θ\right)}{r^{2}}\frac{∂Ψ}{∂θ}+\frac{sin^{2}\left(θ\right)}{r^{2}}\frac{∂^{2}Ψ}{∂θ^{2}}.$$

Combining like terms:

$$\frac{∂^{2}Ψ}{∂x^{2}}=cos^{2}\left(θ\right)\frac{∂^{2}Ψ}{∂r^{2}}+2\frac{cos\left(θ\right)sin\left(θ\right)}{r^{2}}\frac{∂Ψ}{∂θ}-2\frac{cos\left(θ\right)sin\left(θ\right)}{r}\frac{∂^{2}Ψ}{∂r∂θ}+\frac{sin^{2}\left(θ\right)}{r}\frac{∂Ψ}{∂r}+\frac{sin^{2}\left(θ\right)}{r^{2}}\frac{∂^{2}Ψ}{∂θ^{2}}.$$

In a similar fashion one can derive ${∂^{2}Ψ}/{∂y^{2}}$ (this is left for a homework assignment):

$$\frac{∂^{2}Ψ}{∂y^{2}}=sin^{2}\left(θ\right)\frac{∂^{2}Ψ}{∂r^{2}}-2\frac{cos\left(θ\right)sin\left(θ\right)}{r^{2}}\frac{∂Ψ}{∂θ}+2\frac{cos\left(θ\right)sin\left(θ\right)}{r}\frac{∂^{2}Ψ}{∂r∂θ}+\frac{cos^{2}\left(θ\right)}{r}\frac{∂Ψ}{∂r}+\frac{cos^{2}\left(θ\right)}{r^{2}}\frac{∂^{2}Ψ}{∂θ^{2}}.$$

These are added (recall that : $sin^{2}\left(θ\right)+cos^{2}\left(θ\right)=1$)

$$\frac{∂^{2}Ψ}{∂x^{2}}+\frac{∂^{2}Ψ}{∂y^{2}}=\frac{∂^{2}Ψ}{∂r^{2}}+\frac{1}{r}\frac{∂Ψ}{∂r}+\frac{1}{r^{2}}\frac{∂^{2}Ψ}{∂θ^{2}}.$$

This is rewritten as:

$$∇^{2}Ψ=\frac{1}{r}\frac{∂}{∂r}\left(r\frac{∂Ψ}{∂r}\right)+\frac{1}{r^{2}}\frac{∂^{2}Ψ}{∂θ^{2}},$$

or writing as an operator:

$$,$$

which is our final result (i.e. the Laplacian operator in polar coordinates).

Cylindrical Coordinates

The result is easily extended to three dimensional cylindrical coordinates. The Laplacian operator for three dimensional rectangular coordinates is:

$$∇^{2}=\frac{∂^{2}}{∂x^{2}}+\frac{∂^{2}}{∂y^{2}}+\frac{∂^{2}}{∂z^{2}}$$

Recall the conversion formulae:

$$x=rcos\left(θ\right),$$

$$y=rsin\left(θ\right),$$

$$z=z.$$

The $x$ and $y$ conversion are identical to the polar conversions and there is no change to the $z$ variable. Hence the Laplacian operator in cylindrical coordinates is:

$$$$

Homework

1. Derive the expression for $\frac{∂^{2}Ψ}{∂y^{2}}$.
2. If $f\left(r,θ,z\right)=r^{2}\sin(\left(θ\right))+rz^{2}$, find $∇^{2}f$.