
Knowlton

Materials Science and Engineering

Boise State University

Defining operators and taking the complex conjugate with Mathematica

■ Defining an operator

An operator is a mathematical construct that performs a mathematical operation on a function or number. The operator below is called the momentum operator used in quantum mechanics. It takes the first derivative WRT x and multiplies the result by the product between $-i$ and Planck's constant, h , divided by 2π (known as \hbar).

```
g[f_] := i d_x f
```

Let us use the momentum operator on a wave function, $\psi(x)$. We will define a wavefunction, $\psi(x)$, then operate.

```
 $\psi[x_] := A \text{Exp}[i k x]$   
g[ $\psi[x]$ ]
```

```
 $-A e^{i k x} k$ 
```

■ To take the complex conjugate, we actually define an operator.

Remember that the complex conjugate of a function just places a negative sign just prior to any imaginary number.

```
Conj[f_] := f /. Complex[g_, a_] -> Complex[g, -a]
```

Let us take the conjugate of the wavefunction we defined.

```
Conj[ $\psi[x]$ ]
```

```
 $A e^{-i k x}$ 
```

It actually works!