3.4: Operators, Eigenfunctions, Eigenvalues, and Eigenstates

The Laplacian operator is called an operator because it does something to the function that follows: namely, it produces or generates the sum of the three second-derivatives of the function. Of course, this is not done automatically; you must do the work, or remember to use this operator properly in algebraic manipulations. Symbols for operators are often (although not always) denoted by a hat ^ over the symbol, unless the symbol is used exclusively for an operator, e.g. ∇ (del/nabla), or does not involve differentiation, e.g.r for position.

Recall, that we can identify the total energy operator, which is called the Hamiltonian operator, $\hat{H}$, as consisting of the kinetic energy operator plus the potential energy operator.

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \hat{V}(x,y,z) \tag{3.4.1}$$

Using this notation we write the Schrödinger Equation as

$$\hat{H}\psi(x,y,z) = E\psi(x,y,z) \tag{3.4.2}$$

The Hamiltonian

The term Hamiltonian, named after the Irish mathematician Hamilton, comes from the formulation of Classical Mechanics that is based on the total energy,

$$H = T + V \tag{3.4.3}$$

rather than Newton's second law,

$$\vec{F} = m\vec{a} \tag{3.4.4}$$

Equation 3.4.2 says that the Hamiltonian operator operates on the wavefunction to produce the energy, which is a number, (a quantity of Joules), times the wavefunction. Such an equation, where the operator, operating on a function, produces a constant times the function, is called an eigenvalue equation. The function is called an eigenfunction, and the resulting numerical value is called the eigenvalue. Eigen here is the German word meaning self or own.

It is a general principle of Quantum Mechanics that there is an operator for every physical observable. A physical observable is anything that can be measured. If the wavefunction that describes a system is an eigenfunction of an operator, then the value of the associated observable is extracted from the eigenfunction by operating on the eigenfunction with the appropriate operator. The value of the observable for the system is the eigenvalue, and the system is said to be in an eigenstate. Equation 3.4.2 states this principle mathematically for the case of energy as the observable.