Skills to Develop

- Classical-Mechanical Quantities are Represented by Linear Operators in Quantum Mechanics

The bracketed object in the time-independent Schrödinger Equation (in 1D)

\[
\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r}) = E\psi(\vec{r}) \quad \text{label:}\text{3.1.19}
\]

is called an operator. An operator is a generalization of the concept of a function applied to a function. Whereas a function is a rule for turning one number into another, an operator is a rule for turning one function into another. For the time-independent Schrödinger Equation, the operator of relevance is the Hamiltonian operator (often just called the Hamiltonian) and is the most ubiquitous operator in quantum mechanics.

\[
\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})
\]

We often (but not always) indicate that an object is an operator by placing a 'hat' over it, eg, \(\hat{H}\). So time-independent Schrödinger Equation can then be simplified from Equation \ref{3.1.19} to

\[
\hat{H} \psi(\vec{r}) = E\psi(\vec{r}) \quad \text{label:simple}
\]

Equation \ref{simple} says that the Hamiltonian operator operates on the wavefunction to produce the energy, which is a number, (a quantity or observable), 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. We will discuss this in detail in later Sections.

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**Fundamental Properties of Operators**

Most properties of operators are straightforward, but they are summarized below for completeness.

The sum and difference of two operators \(\hat{A}\) and \(\hat{B}\) are given by

\[
(\hat{A} \pm \hat{B}) f = \hat{A} f \pm \hat{B} f
\]

The product of two operators is defined by

\[
\hat{A} \hat{B} f \equiv \hat{A} [\hat{B} f]
\]

Two operators are equal if

\[
\hat{A} f = \hat{B} f
\]

for all functions \(f\).

The identity operator \(\hat{1}\) does nothing (or multiplies by 1)

\[
\hat{1} f = f
\]
The associative law holds for operators
\[ \hat{A}(\hat{B}\hat{C}) = (\hat{A}\hat{B})\hat{C} \]

The commutative law does not generally hold for operators. In general,
\[ \hat{A}\hat{B} \neq \hat{B}\hat{A} \]

It is convenient to define the commutator of \( \hat{A} \) and \( \hat{B} \)
\[ [\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A} \]

Note that the order matters, so that
\[ [[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}] \]

If \( \hat{A} \) and \( \hat{B} \) commute, then
\[ [[\hat{A}, \hat{B}] = 0 \]

The \( n \)-th power of an operator \( \hat{A}^n \) is defined as \( n \) successive applications of the operator, e.g.
\[ \hat{A}^2 f = \hat{A}\hat{A} f \]

**Definition: The Momentum Operator in 3D**

Equation 3.1.11 from Section 3.1 implies that the operator for the \( x \)-component of momentum can be written
\[ \hat{p}_x = -i\hbar \frac{\partial}{\partial x} \]

and by analogy, we must have the other two operators representing momenta in the other dimensions.
\[ \hat{p}_y = -i\hbar \frac{\partial}{\partial y} \]

and
\[ \hat{p}_z = -i\hbar \frac{\partial}{\partial z} \]

**Linear Operators**

The action of an operator that turns the function \( f(x) \) into the function \( g(x) \) is represented by
\[ \hat{A} f(x) = g(x) \]

The most common kind of operator encountered are linear operators which satisfies the following two conditions:
\[ \underset{\text{Condition A}}{\hat{O}(f(x)+g(x)) = \hat{O}f(x)+\hat{O}g(x)} \]
and

\[
\overset{\text{Condition B}}{\hat{O}cf(x) = c \hat{O}f(x)} \label{3.2.2b}
\]

where

- \((\hat{O})\) is a linear operator,
- \((c)\) is a constant that can be a complex number \((c = a + ib)\), and
- \((f(x))\) and \((g(x))\) are functions of \((x)\)

If an operator fails to satisfy the conditions in either Equations \ref{3.2.2a} or \ref{3.2.2b}, then it is not a linear operator.

Example \(\PageIndex{1}\)

Is the differentiation operator \(\left(\frac{d}{dx}\right)\) linear?

**Solution**

To confirm is an operator is linear, both conditions in Equation \ref{3.2.2b} must be demonstrated.

Condition A (Equation \ref{3.2.2a}):

\[
\hat{O}(f(x)+g(x)) = \frac{d}{dx} \left( f(x)+g(x) \right) \quad \checkmark
\]

Condition A is confirmed. Does Condition B (Equation \ref{3.2.2b}) hold?

\[
\hat{O}cf(x) = \frac{d}{dx} c f(x) = c \frac{d}{dx} f(x) = c \hat{O}f(x) \quad \checkmark
\]

Yes. The differentiation operator is a linear operator

Exercise \(\PageIndex{1}\)

Confirm if the square root operator \(\sqrt{f(x)}\) linear or not?

**Answer**

To confirm is an operator is linear, both conditions in Equations \ref{3.2.2a} and \ref{3.2.2b} must be demonstrated. Let's look first at Condition B.

Does Condition B (Equation \ref{3.2.2b}) hold?
\[ \hat{O}cf(x) = c\hat{O}{ f(x) } \] 
\[ \sqrt{c f(x) } \neq c\sqrt{f(x)} \]

Condition B does not hold, therefore the square root operator is not linear.

The most operators encountered in quantum mechanics are **linear operators**.

### Hermitian Operators

An important property of operators is suggested by considering the Hamiltonian for the particle in a box:

\[ \hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \]  \hfill (1)

Let \( f(x) \) and \( g(x) \) be arbitrary functions which obey the same boundary values as the eigenfunctions of \( \hat{H} \) (e.g., they vanish at \( x = 0 \)) and \( x = a \)'). Consider the integral

\[ \int_0^a f(x) \hat{H} g(x) \, dx = -\frac{\hbar^2}{2m} \int_0^a f(x) g''(x) \, dx \]  \hfill (2)

Now, using **integration by parts**,  

\[ \int_0^a f(x) g''(x) \, dx = - \int_0^a f'(x) g'(x) \, dx + [f(x) g'(x)]_0^a \]  \hfill (3)

The boundary terms vanish by the assumed conditions on \( f \) and \( g \). A second integration by parts transforms Equation (3) to

\[ \int_0^a f''(x) g(x) \, dx + [f'(x) g(x)]_0^a \]

It follows therefore that

\[ \int_0^a f(x) \hat{H} g(x) \, dx = \int_0^a g(x) \hat{H} f(x) \, dx \]  \hfill (4)

An obvious generalization for complex functions will read

\[ \int_0^a f^*(x) \hat{H} g(x) \, dx = \int_0^a g^*(x) \hat{H} f(x) \, dx \]  \hfill (5)

In mathematical terminology, an operator \( \hat{A} \) for which

\[ \int \! f^* \hat{A} g \, d\tau = \left( \int \! g^* \hat{A} f \, d\tau \right)^* \]

for all functions \( f \) and \( g \) which obey specified boundary conditions is classified as **hermitian** or **self-adjoint**. Evidently, the Hamiltonian is a hermitian operator. It is postulated that **all** quantum-mechanical operators that represent dynamical variables are hermitian.
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