

4.6 Wave Mechanics

In this section, we generalize the concepts we have learned in the previous sections. The goal here is to give a broader description of quantum mechanics in terms of wave functions that are solutions to the Schroedinger Equation.

In classical mechanics the particle state is determined by its position and momentum and the state evolution is determined by Newton's law. In quantum mechanics the particle state is completely described by its wave function and the state evolution is determined by the Schroedinger equation.

The wave function as a complete description of the particle enables us to compute expected values of physical quantities of the particle when a corresponding measurement is performed. The measurement results are real numbers, like the energy, or position or momentum the particle has in this state. The physically measurable quantities are called observables. In classical mechanics these observables or real variables like x for position, p for momentum or functions thereof, like the energy, which is called the Hamiltonian $H(p, x) = \frac{p^2}{2m} + V(x)$ in classical mechanics. For simplicity, we state the results only for one-dimensional systems but it is straight forward to extend these results to multi-dimensional systems. In quantum mechanics these observables become operators:

$$x \quad : \quad \text{position operator} \quad (4.133)$$

$$p = \frac{\hbar}{j} \frac{\partial}{\partial x} \quad : \quad \text{momentum operator} \quad (4.134)$$

$$H(p, x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \quad : \quad \text{Hamiltonian operator} \quad (4.135)$$

If we carry out measurements of these observables, the result is a real number in each measurement and after many measurements on identical systems we can make a statistics of these measurements and the statistics is completely described by the moments of the observable.

4.6.1 Position Statistics

The statistical interpretation of quantum mechanics enables us to compute the expected value of the position operator or any of its moments according

to

$$\langle x \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) x \Psi(x, t) dx \quad (4.136)$$

$$\langle x^m \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) x^m \Psi(x, t) dx \quad (4.137)$$

The expectation value of functions of operators can always be evaluated by defining the operator by its Taylor expansion

$$\begin{aligned} \langle f(x) \rangle &= \int_{-\infty}^{\infty} \Psi^*(x, t) f(x) \Psi(x, t) dx \quad (4.138) \\ &= \left\langle \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(0) x^n \right\rangle \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(0) \left\langle \int_{-\infty}^{\infty} \Psi^*(x, t) x^n \Psi(x, t) dx \right\rangle \end{aligned}$$

4.6.2 Momentum Statistics

The momentum statistics is then

$$\langle p \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) \frac{\hbar}{j} \frac{\partial}{\partial x} \Psi(x, t) dx \quad (4.139)$$

which can be written in terms of the wave function in the wave number space, which we define now for symmetry reasons as the Fourier transform of the wave function where the 2π is symmetrically distributed between Fourier and inverse Fourier transform

$$\phi(k, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x, t) e^{-jkx} dx, \quad (4.140)$$

$$\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k, t) e^{jkx} dk. \quad (4.141)$$

Using the differentiation theorem of the Fourier transform and the generalized Parseval relation

$$\int_{-\infty}^{\infty} \phi_1^*(k) \phi_2(k) dk = \int_{-\infty}^{\infty} \Psi_1^*(x) \Psi_2(x) dx \quad (4.142)$$

we find

$$\langle p \rangle = \int_{-\infty}^{\infty} \phi^*(k, t) \hbar k \phi(k, t) dk \quad (4.143)$$

$$= \int_{-\infty}^{\infty} \hbar k |\phi(k, t)|^2 dk. \quad (4.144)$$

The introduction of the symmetrically defined expectation value of an operator according Eq.(4.136), where x can stand for any operator can be carried out using the wave function in the position space or the wave number space using the corresponding representation of the wave function and of the operator.

4.6.3 Energy Statistics

The analysis for the measurement of position or moment carries over to every observable in an analogous way. Thus the expectation value of the energy is

$$\langle H(x, p) \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) H(x, p) \Psi(x, t) dx \quad (4.145)$$

$$= \int_{-\infty}^{\infty} \Psi^*(x, t) \left(-\frac{1}{2m\hbar^2} \frac{\partial^2}{\partial x^2} + V(x) \right) \Psi(x, t) dx \quad (4.146)$$

If the system is in an energy eigenstate, i.e.

$$\Psi(x, t) = \psi_n(x) e^{j\omega_n t} \quad (4.147)$$

with

$$H(x, p) \psi_n(x) = E_n \psi_n(x), \quad (4.148)$$

we obtain

$$\langle H(x, p) \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) E_n \Psi(x, t) dx = E_n. \quad (4.149)$$

If the system is in a superposition of energy eigenstates

$$\Psi(x, t) = \sum_{n=0}^{\infty} c_n \psi_n(x) e^{j\omega_n t}. \quad (4.150)$$

we obtain

$$\langle H(x, p) \rangle = \sum_{n=0}^{\infty} E_n |c_n|^2. \quad (4.151)$$

4.6.4 Arbitrary Observable

There may also occur observables that are not simple to translate from the classical to the quantum domain, such as the product

$$p_{cl} \cdot x_{cl} = x_{cl} \cdot p_{cl} \quad (4.152)$$

Classically it does not matter which variable comes first. However, if we transfer this expression into quantum mechanics, the corresponding operator depends on the ordering, for example

$$p_{qm} \cdot x_{qm} \Psi(x, t) = \frac{\hbar}{j} \frac{\partial}{\partial x} (x \Psi(x, t)) = \quad (4.153)$$

$$= \frac{\hbar}{j} \Psi(x, t) + \frac{\hbar}{j} x \frac{\partial}{\partial x} \Psi(x, t), \quad (4.154)$$

$$= \left(\frac{\hbar}{j} + x_{qm} \cdot p_{qm} \right) \Psi(x, t). \quad (4.155)$$

The decision of which expression represents the correct quantum mechanical operator or eventually even a linear combination of the possible expressions, has to be based on a close examination of the actual measurement apparatus that would measure the corresponding observable. Finally, the expression also has to deliver results that are in agreement with experimental findings.

If we have an operator that is a function of x and p and we have decided on a unique expression in terms of a power expansion in x and p

$$g(x, p) \rightarrow g_{op}(x, \frac{\hbar}{j} \frac{\partial}{\partial x}) \quad (4.156)$$

then we can compute its expected value either in the space domain or the wave number domain

$$\langle g_{op} \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) g_{op}(x, \frac{\hbar}{j} \frac{\partial}{\partial x}) \Psi(x, t) dx \quad (4.157)$$

$$= \int_{-\infty}^{\infty} \phi^*(k, t) g_{op}(j \frac{\partial}{\partial k}, \hbar k) \phi(k, t) dk \quad (4.158)$$

That is this operator can be represented either in real space or in k-space as $g_{op}(x, \frac{\hbar}{j} \frac{\partial}{\partial x})$ or $g_{op}(j \frac{\partial}{\partial k}, \hbar k)$.

4.6.5 Eigenfunctions and Eigenvalues of Operators

A differential operator has in general eigenfunctions and corresponding eigenvalues

$$g_{op}(x, \frac{\hbar}{j} \frac{\partial}{\partial x}) \psi_n(x) = g_n \psi_n(x), \quad (4.159)$$

where g_n is the eigenvalue to the eigenfunction $\psi_n(x)$. An example for a differential operator is the Hamiltonian operator describing a particle moving in a potential

$$H_{op} = -\frac{1}{2m\hbar^2} \frac{\partial^2}{\partial x^2} + V(x) \quad (4.160)$$

the corresponding eigenvalue equation is the stationary Schroedinger Equation

$$H_{op}\psi_n(x) = E_n\psi_n(x). \quad (4.161)$$

Thus the energy levels of a quantum system are the eigenvalues of the corresponding Hamiltonian operator.

The operator for which

$$\int \psi_n^*(x) (H_{op}\psi_m(x)) dx = \int (H_{op}\psi_n(x))^* \psi_m(x) dx, \quad (4.162)$$

for arbitrary wave functions ψ_n and ψ_m is called a hermitian operation. From this equation we find immediately that the expected values of a hermitian operator are real, which also has the consequence that the eigenvalues of hermitian operators are real. This is important since operators that represent observables must have real expected values and real eigenvalues since these are results of physical measurements, which are real. Thus observables are represented by hermitian operators. This is easy to prove. Let's assume we have found two eigenfunctions and the corresponding eigen values

$$g_{op}\psi_m = g_m\psi_m, \quad (4.163)$$

$$g_{op}\psi_n = g_n\psi_n. \quad (4.164)$$

Then

$$\int \psi_n^* g_{op}\psi_m dx = g_m \int \psi_n^* \psi_m. \quad (4.165)$$

By taking advantage of the fact that the operator is hermitian we can also write

$$\int \psi_n^* g_{op} \psi_m dx = \int (g_{op} \psi_n)^* \psi_m dx = g_n^* \int \psi_n^* \psi_m dx \quad (4.166)$$

The right sides of Eqs.(4.165) and (4.166) must be equal

$$(g_m - g_n^*) \int \psi_n^* \psi_m dx = 0 \quad (4.167)$$

If $n = m$ the integral can not vanish and Eq.(4.167) enforces $g_n = g_n^*$, i.e. the corresponding eigenvalues are real. If $n \neq m$ and the corresponding eigenvalues are not degenerate, i.e. different eigenfunctions have different eigenvalues, then Eq.(4.167) enforces that the eigenfunctions are orthogonal to each other

$$\int \psi_n^* \psi_m dx = 0, \text{ for } n \neq m. \quad (4.168)$$

Thus, if there is no degeneracy, the eigenfunctions of a hermitian operator are orthogonal to each other. If there is degeneracy, one can always choose an orthogonal set of eigenfunctions. If the eigenfunctions are properly normalized $\int \psi_n^* \psi_n dx = 1$, then the eigenfunctions build an orthonormal system

$$\int \psi_n^* \psi_m dx = \delta_{nm}, \quad (4.169)$$

and are complete, i.e. any arbitrary function $f(x)$ can be expressed as a superposition of the orthonormal basis functions $\psi_n(x)$

$$f(x) = \sum_{n=0}^{\infty} c_n \psi_n(x). \quad (4.170)$$

Thus we can freely change the basis in which we describe a certain physical problem. To account fully for this fact, we no longer wish to use wave mechanics, ie. express the wave function as a function in position space or in k -space. Instead we will utilize a vector in an abstract function space, i.e. a Hilbert space. In this way, we can formulate a physical problem, without using a fixed representation for the state of the system (wave function) and the corresponding operator representations. This description enables us to make full use of the mathematical structure of Hilbert spaces and the algebraic properties of operators.

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