1.2: Wavefunctions

The eigenfunctions of a quantum mechanical operator depend on the coordinates upon which the operator acts; these functions are called wavefunctions

In addition to operators corresponding to each physically measurable quantity, quantum mechanics describes the state of the system in terms of a wavefunction Ψ that is a function of the coordinates $\{q_j\}$ and of time t. The function $|\Psi(q_j,t)|^2 = \Psi^*\Psi$ gives the probability density for observing the coordinates at the values q_j at time t. For a many-particle system such as the H_2O molecule, the wavefunction depends on many coordinates. For the H_2O example, it depends on the x, y, and z (or r,q, and f) coordinates of the ten electrons and the x, y, and z (or r,q, and f) coordinates of the oxygen nucleus and of the two protons; a total of thirty-nine coordinates appear in Ψ.

In classical mechanics, the coordinates qj and their corresponding momenta p_j are functions of time. The state of the system is then described by specifying q_j (t) and p_j (t). In quantum mechanics, the concept that qj is known as a function of time is replaced by the concept of the probability density for finding q_j at a particular value at a particular time t: $|\Psi(q_j,t)|^2$. Knowledge of the corresponding momenta as functions of time is also relinquished in quantum mechanics; again, only knowledge of the probability density for finding p_j with any particular value at a particular time t remains.