


## 5.S: Translational States (Summary)

In this chapter we applied the principles of quantum mechanics to the simplest physical system, a free particle in one dimension, which could be an electron, an atom, or a molecule. We wrote the Schrödinger equation for the system and then solved this equation to obtain the wavefunctions,  $\psi_k(x)$ , describing the system. Each wavefunction is identified by the magnitude of the wave vector,  $k$ , as a subscript. We observed that the wavefunctions are not quantized because there are no boundary conditions for this system. By “not quantized,” we mean that the wave vector, momentum, and energy can have any values. We determined the constants of integration for our solutions by using the normalization condition. By using the wavefunction and the momentum operator to obtain the momentum of the particle, we discovered that the momentum was related to the wave vector and wavelength just as Compton and de Broglie proposed. Note that the momentum and energy of the free particle are related just as they are classically. The position of the particle is completely undetermined by the wavefunction because the momentum is given exactly. The particle could be anywhere. This relationship between momentum and position is a manifestation of the Heisenberg Uncertainty Principle. The momentum is known exactly because the wavefunction is an eigenfunction of the momentum operator.

The concepts of overlap, orthogonality, and linear combination or superposition of functions appeared in the discussion. These concepts will be useful later when we discuss bonding and the mathematical representations of bonding in semi-empirical and ab initio molecular orbital theories. Linear combinations of atomic orbitals and other functions are used to describe bonds in molecules, and the overlap and orthogonality of these functions are important there.

**Exercise 5.S. 14** Complete the table below. For an example of a completed table, see the overview table at the end of Chapter 4.

Overview of key concepts and equations for the free particle

|                               |   |
|-------------------------------|---|
| Potential energy              | $V =$   |
| Hamiltonian                   |  |
| Wavefunctions                 | $\Psi =$  |
| Quantum Numbers               |   |
| Energies                      | $E =$   |
| Spectroscopic Selection Rules |   |
| Angular Momentum Properties   |   |

### Contributors and Attributions

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