 Brief review of the Schrödinger equation

The Schrödinger equation has the general form: \[ H \psi = E \cdot \psi \]

H = Hamiltonian = Energy Operator
E = Energy Eigenvalue = Energy Level
\( \psi(r) \) = Wave Function

A quantum mechanical state is characterized by its quantum numbers (energy, spin, ...)
An energy level can contain several states (with different spin, ...). The number of states per energy level is the degeneracy.

One-electron Schrödinger equation: \[ H(r,p) = p^2/2m + V(r) \]

\( p = -i \hbar \partial / \partial r \) = Momentum Operator

\[ V(r) = \text{Potential energy} \]
\[ = \text{Coulomb energy between electrons and } H^+ \text{ ions} \]

(Shown schematically for \( H_2 \))

Two-electron Schrödinger equation:

\[ H(r_1,r_2,p_1,p_2) = p_1^2/2m + p_2^2/2m + V(r_1) + V(r_2) + e^2/4\pi\varepsilon_0 \cdot \frac{1}{|r_1-r_2|} \]

\( \text{Kinetic energy} \quad \text{Potential energy} \quad e^-e^- \text{Coulomb energy} \)

Position of electron 1: \( r_1 \)
Position of electron 2: \( r_2 \)
Momentum operator of electron 1: \( p_1 = -i \hbar \partial / \partial r_1 \)
Momentum operator of electron 2: \( p_2 = -i \hbar \partial / \partial r_2 \)

The \( H^+H^+ \) Coulomb energy \( e^2/4\pi\varepsilon_0 \cdot \frac{1}{a} \) is independent of \( r_1, r_2 \) (a = bond length).
This constant needs to be added to the energy E for obtaining the total energy of electrons and ions.
Angular Momentum

Orbital Angular Momentum: \( \mathbf{L} \) (vectors in bold)

Spin Angular Momentum: \( \mathbf{S} \)

Total Angular Momentum: \( \mathbf{J} = \mathbf{L} + \mathbf{S} \)

Angular momentum quantum numbers \( j, m_j \):

\[
\begin{align*}
  j^2 &= \hbar^2 \cdot j(j+1) \\
  j_z &= \hbar \cdot m_j \\
  m_j &= -j, -j+1, \ldots, +j \\
  \text{with } (2j+1)
\end{align*}
\]

\( j = L \):
- \( l = 0, 1, 2, 3, \ldots \)
  - \( s, p, d, f, \ldots \)

\( j = S \):
- \( s = 0, \frac{1}{2}, 1, \ldots \)
  - \( (2s+1) \) singlet, doublet, triplet, …

Addition of two angular momenta:

\( \mathbf{j} = \mathbf{j}_1 + \mathbf{j}_2 \) \( j = |j_1 - j_2|, \ldots, j_1 + j_2 \)