Atoms

Byungjoon Min

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Department of Physics, Chungbuk National University

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The Hamiltonian of a neutral atom with Z electrons is

$$H = \sum_{j=1}^{Z} \left[-\frac{\hbar^2}{2m} \nabla_j^2 - \left(\frac{1}{4\pi\epsilon_0} \right) \frac{Ze^2}{r_j} \right] + \frac{1}{2} \left(\frac{1}{4\pi\epsilon_0} \right) \sum_{j \neq k}^{Z} \frac{e^2}{|r_j - r_k|}.$$

We need to solve $H\psi = E\psi$, and then have the complete state (position and spin)

$$\psi(r_1, r_2, \cdots, r_Z)\chi(s_1, s_2, \cdots, s_Z).$$

Unfortunately, the equation with the Hamiltonian have not been solved exactly except $Z = 1$ (hydrogen). Therefore, we need approximation methods.

The Periodic Table

To first approximation (ignoring the mutual repulsion between electrons), the individual electrons occupy (n, l, m) states, called "orbitals". Because of spins, there can be two possible state (up and down) for each orbital.

$(1, 0, 0)$ corresponds to hydrogen $(Z = 1)$ and helium $(Z = 2)$. Then, next electrons put into $n = 2$ shell. Due to the screening, $(2, 0, 0)$ corresponds to $Z = 3$ and 4. $(2, 1, 1)$, $(2, 1, 0)$, $(2, 1, -1)$ correspond to $Z = 5, 6, 7, 8, 9, 10$. And so on.

The Periodic Table

- Orbitals (n, l, m)
- n: shell number (principle quantum number)
- l: 0,1,2,$\cdots$,n (azimuthal quantum number)
- l: s (sharp, l=0), p (principal, l=1), d (diffuse, l=2), f (fundamental, l=3), g, h, i, k, l, $\cdots$.
- m: -l,-l+1,$\cdots$,l-1,l (magnetic quantum number)