

Useful Identities in Atomic Physics

The quantum numbers of the energy eigenstates of the non-relativistic hydrogenoid atom are: n (energy), ℓ (angular momentum) and m (z projection of angular momentum). $\langle \cdot \rangle$ means average over *energy* eigenstates.

Scales, Constants and Special Values of Hydrogenoid Wave Functions [1]

Energies for the Coulomb Potential ($V(\mathbf{r}) = -\frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r}$) are $E_n = -\frac{\mu}{2n^2} \left(\frac{Ze^2}{4\pi\epsilon_0\hbar} \right)^2 = -\frac{e^2}{4\pi\epsilon_0 a_0} \frac{Z^2}{2n^2} = -\frac{1}{2} \mu c^2 \frac{(Z\alpha)^2}{n^2}$.

Fine structure constant: $\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c}$. Bohr radius: $a_0 = 4\pi\epsilon_0\hbar^2/(\mu e^2)$. $|\psi_{n\ell m}(0)|^2 = \frac{Z^3}{\pi a_0^3 n^3} \delta_\ell^0 \delta_m^0$.

Expected Values, the Virial Theorem and the Gamma Function [2, 3]

Virial Theorem (valid for *any* potential): If $H = T(\mathbf{p}) + V(\mathbf{r})$ and $T(\mathbf{p}) = \frac{\mathbf{p}^2}{2\mu}$ then $2\langle T \rangle = \langle \mathbf{r} \cdot \nabla V \rangle$.

Expectation values for the Coulomb potential: $\langle \frac{1}{r} \rangle = \frac{Z}{a_0 n^2}$, $\langle \frac{1}{r^2} \rangle = \frac{Z^2}{a_0^2 n^3 (\ell + 1/2)}$.

Recursion Relation: $0 = \frac{s}{4} [(2\ell + 1)^2 - s^2] \left(\frac{a_0}{Z} \right)^2 \langle r^{s-2} \rangle - (2s + 1) \left(\frac{a_0}{Z} \right) \langle r^{s-1} \rangle + \frac{s+1}{n^2} \langle r^s \rangle$.

$\Gamma(z) = \int_0^\infty t^{z-1} e^{-t} dt$, $\Gamma(n+1) = n!$, $\Gamma(1-z)\Gamma(z) = \frac{\pi}{\sin(\pi z)}$, $\Gamma(z)\Gamma\left(z + \frac{1}{2}\right) = 2^{1-2z} \sqrt{\pi} \Gamma(2z)$.

Spherical Harmonics, Wigner 3j Symbols and Clebsch – Gordan Coefficients [4]

$\int_0^{2\pi} d\phi \int_0^\pi \sin\theta d\theta \mathcal{Y}_{\ell_1}^{m_1}(\theta, \phi) \mathcal{Y}_{\ell_2}^{m_2}(\theta, \phi) \mathcal{Y}_{\ell_3}^{m_3}(\theta, \phi) = \sqrt{\frac{(2\ell_1+1)(2\ell_2+1)(2\ell_3+1)}{4\pi}} \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$.

Wigner 3j — Clebsch–Gordan (CG) relation: $\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \equiv \frac{(-1)^{j_1-j_2-m_3}}{\sqrt{2j_3+1}} \langle j_1 m_1 j_2 m_2 | j_3 -m_3 \rangle$.

Selection rules for Wigner 3j Symbol $\begin{pmatrix} \ell_1 & \ell_2 & L \\ m_1 & m_2 & -M \end{pmatrix}$ (they are identical to CG Selection Rules):

$$-\ell_i \leq m_i \leq \ell_i, \quad m_1 + m_2 = M, \quad |\ell_1 - \ell_2| \leq L \leq \ell_1 + \ell_2, \quad \ell_1 + \ell_2 + L \in \mathbb{Z}.$$

Spherical components of a cartesian vector $\vec{e} = (e_x, e_y, e_z)$: $e_{\pm 1} = \mp \frac{1}{\sqrt{2}} (e_x \pm i e_y)$ and $e_0 = e_z$.

Ladder Operators: $\hat{\ell}_\pm \equiv \hat{\ell}_x \pm i \hat{\ell}_y$. $\hat{\ell}_\pm |\ell, m\rangle = \hbar \sqrt{\ell(\ell+1) - m(m \pm 1)} |\ell, m \pm 1\rangle$.

References

- [1] P. Ewart, *Atomic Physics Lecture notes* <https://users.physics.ox.ac.uk/~ewart/>
- [2] S. Jeon, *Lecture Notes for Quantum Physics II*. <http://www.physics.mcgill.ca/~jeon/Phys457/>
- [3] E. W. Weisstein, “Gamma Function.” <http://mathworld.wolfram.com/GammaFunction.html>
- [4] E. W. Weisstein, “Wigner 3j-Symbol.” <http://mathworld.wolfram.com/Wigner3j-Symbol.html>