

# Useful Identities in Atomic Physics

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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:  $a_0 = 4\pi\epsilon_0\hbar^2/(\mu e^2)$ .  $|\psi_{nlm}(0)|^2 = \frac{Z^3}{\pi a_0^3 n^3} \delta_l^0 \delta_m^0$ .

## 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:  $\langle \frac{1}{r} \rangle = \frac{Z}{a_0 n^2}$ ,  $\langle \frac{1}{r^2} \rangle = \frac{Z^2}{a_0^2 n^3 (l+1/2)}$ .

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

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

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

$\int_0^{2\pi} d\phi \int_0^\pi \sin\theta d\theta \mathcal{Y}_{l_1}^{m_1}(\theta, \phi) \mathcal{Y}_{l_2}^{m_2}(\theta, \phi) \mathcal{Y}_{l_3}^{m_3}(\theta, \phi) = \sqrt{\frac{(2l_1+1)(2l_2+1)(2l_3+1)}{4\pi}} \begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$ .

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  $\begin{pmatrix} l_1 & l_2 & L \\ m_1 & m_2 & -M \end{pmatrix}$  (they are identical to CG Selection Rules):

$$-l_i \leq m_i \leq l_i, \quad m_1 + m_2 = M, \quad |l_1 - l_2| \leq L \leq l_1 + l_2 \quad l_1 + l_2 + L \in \mathbb{Z}.$$

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

## 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>