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

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

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

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

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

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

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):

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

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

Ladder Operators: $\hat{\ell}_\pm \equiv \hat{\ell}_x \pm i\hat{\ell}_y$. $\quad \hat{\ell}_\pm|\ell,m\rangle = \hbar\sqrt{\ell(\ell+1) - m(m\pm1)}|\ell, m\pm1\rangle$.

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] NIST Digital Library of Mathematical Functions. https://dlmf.nist.gov/, Release 1.2.3 of 2024-12-15.