Useful Identities in Atomic Physics

Nicolás Quesada
Instituto de Física, Universidad de Antioquia

Notation and Conventions

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

Scales Constants and Special Values of Hydrogenoid Wave Functions

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

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

Expected Values, the Virial Theorem and the Gamma Function

Virial Theorem: If $H = T(\mathbf{p}) + V(\mathbf{r})$ and $T(\mathbf{p}) = \mathbf{p}^2/2m$ then $2\langle T\rangle = \langle \mathbf{r}\cdot\nabla V\rangle$

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

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

Definition: $\Gamma(z) = \int_0^\infty t^{z-1}e^{-t}\,dt$.

Identities: $\Gamma(n+1) = n!$, $\Gamma(1-z)\,\Gamma(z) = \frac{\pi}{\sin(\pi z)}$, $\Gamma(z)\,\Gamma\left(z+\frac{1}{2}\right) = 2^{1-2z}\sqrt{\pi}\,\Gamma(2z)$.

Integrals of 3 Spherical Harmonics, Wigner 3j Symbols and Clebsch Gordan Coefficients

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

Wigner 3-j Clebsch Gordan 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 3-j Symbol $\begin{pmatrix} l_1 & l_2 & L \\ m_1 & m_2 & -M\end{pmatrix}$ (they are identical to C-G Selection Rules):

$m_i \in \{-l_i, -l_i+1, ..., l_i-1, l_i\} \quad m_1 + m_2 = M \quad |l_1 - l_2| \leqslant L \leqslant l_1 + l_2 \quad l_1 + l_2 + L \in \mathbb{N}$

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

References

[1] B.H. Bransden, C.J. Joachain *Physics of Atoms and Molecules*, Prentice Hall.

[2] G.B. Arfken, H.J. Weber *Mathematical Methods for Physicists*, Harcourt Academic Press.

[3] Weisstein, Eric W. "Wigner 3j-Symbol." From MathWorld–A Wolfram Web Resource. http://mathworld.wolfram.com/Wigner3j-Symbol.html