PERIODIC TABLE

Atomic Properties of the Elements

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Standard Reference Data Group
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Frequently used fundamental physical constants

For the most accurate values of these and other constants, visit physics.nist.gov/constants

1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ^{133}Cs

speed of light in vacuum	c	299 792 458 m s^{-1}	(exact)
Planck constant	h	6.6261×10^{-34} J s	($\hbar = h/2\pi$)
elementary charge	e	1.6022×10^{-19} C	
electron mass	m_e	9.1094×10^{-31} kg	
	$m_e c^2$	0.5110 MeV	
proton mass	m_p	1.6726×10^{-27} kg	
fine-structure constant	α	1/137.036	
Rydberg constant	R_∞	10 973 732 m^{-1}	
	$R_\infty c$	$3.289\,842 \times 10^{15}$ Hz	
	$R_\infty hc$	13.6057 eV	
Boltzmann constant	k	1.3807×10^{-23} J K^{-1}	

Solids
Liquids
Gases
Artificially Prepared

Group	1 IA	2 IIA	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8	9 VIII	10	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
1	1 $^2S_{1/2}$ **H** Hydrogen 1.00794 1s 13.5984																	2 $^1S_0$ **He** Helium 4.002602 $1s^2$ 24.5874
2	3 $^2S_{1/2}$ **Li** Lithium 6.941 $1s^2 2s$ 5.3917	4 $^1S_0$ **Be** Beryllium 9.012182 $1s^2 2s^2$ 9.3227											5 $^2P^o_{1/2}$ **B** Boron 10.811 $1s^2 2s^2 2p$ 8.2980	6 $^3P_0$ **C** Carbon 12.0107 $1s^2 2s^2 2p^2$ 11.2603	7 $^4S^o_{3/2}$ **N** Nitrogen 14.0067 $1s^2 2s^2 2p^3$ 14.5341	8 $^3P_2$ **O** Oxygen 15.9994 $1s^2 2s^2 2p^4$ 13.6181	9 $^2P^o_{3/2}$ **F** Fluorine 18.9984032 $1s^2 2s^2 2p^5$ 17.4228	10 $^1S_0$ **Ne** Neon 20.1797 $1s^2 2s^2 2p^6$ 21.5645
3	11 $^2S_{1/2}$ **Na** Sodium 22.989770 [Ne]3s 5.1391	12 $^1S_0$ **Mg** Magnesium 24.3050 $[Ne]3s^2$ 7.6462											13 $^2P^o_{1/2}$ **Al** Aluminum 26.981538 $[Ne]3s^2 3p$ 5.9858	14 $^3P_0$ **Si** Silicon 28.0855 $[Ne]3s^2 3p^2$ 8.1517	15 $^4S^o_{3/2}$ **P** Phosphorus 30.973761 $[Ne]3s^2 3p^3$ 10.4867	16 $^3P_2$ **S** Sulfur 32.065 $[Ne]3s^2 3p^4$ 10.3600	17 $^2P^o_{3/2}$ **Cl** Chlorine 35.453 $[Ne]3s^2 3p^5$ 12.9676	18 $^1S_0$ **Ar** Argon 39.948 $[Ne]3s^2 3p^6$ 15.7596
4	19 $^2S_{1/2}$ **K** Potassium 39.0983 [Ar]4s 4.3407	20 $^1S_0$ **Ca** Calcium 40.078 $[Ar]4s^2$ 6.1132	21 $^2D_{3/2}$ **Sc** Scandium 44.955910 $[Ar]3d4s^2$ 6.5615	22 $^3F_2$ **Ti** Titanium 47.867 $[Ar]3d^2 4s^2$ 6.8281	23 $^4F_{3/2}$ **V** Vanadium 50.9415 $[Ar]3d^3 4s^2$ 6.7462	24 $^7S_3$ **Cr** Chromium 51.9961 $[Ar]3d^5 4s$ 6.7665	25 $^6S_{5/2}$ **Mn** Manganese 54.938049 $[Ar]3d^5 4s^2$ 7.4340	26 $^5D_4$ **Fe** Iron 55.845 $[Ar]3d^6 4s^2$ 7.9024	27 $^4F_{9/2}$ **Co** Cobalt 58.933200 $[Ar]3d^7 4s^2$ 7.8810	28 $^3F_4$ **Ni** Nickel 58.6934 $[Ar]3d^8 4s^2$ 7.6398	29 $^2S_{1/2}$ **Cu** Copper 63.546 $[Ar]3d^{10} 4s$ 7.7264	30 $^1S_0$ **Zn** Zinc 65.409 $[Ar]3d^{10} 4s^2$ 9.3942	31 $^2P^o_{1/2}$ **Ga** Gallium 69.723 $[Ar]3d^{10} 4s^2 4p$ 5.9993	32 $^3P_0$ **Ge** Germanium 72.64 $[Ar]3d^{10} 4s^2 4p^2$ 7.8994	33 $^4S^o_{3/2}$ **As** Arsenic 74.92160 $[Ar]3d^{10} 4s^2 4p^3$ 9.7886	34 $^3P_2$ **Se** Selenium 78.96 $[Ar]3d^{10} 4s^2 4p^4$ 9.7524	35 $^2P^o_{3/2}$ **Br** Bromine 79.904 $[Ar]3d^{10} 4s^2 4p^5$ 11.8138	36 $^1S_0$ **Kr** Krypton 83.798 $[Ar]3d^{10} 4s^2 4p^6$ 13.9996
5	37 $^2S_{1/2}$ **Rb** Rubidium 85.4678 [Kr]5s 4.1771	38 $^1S_0$ **Sr** Strontium 87.62 $[Kr]5s^2$ 5.6949	39 $^2D_{3/2}$ **Y** Yttrium 88.90585 $[Kr]4d5s^2$ 6.2173	40 $^3F_2$ **Zr** Zirconium 91.224 $[Kr]4d^2 5s^2$ 6.6339	41 $^6D_{1/2}$ **Nb** Niobium 92.90638 $[Kr]4d^4 5s$ 6.7589	42 $^7S_3$ **Mo** Molybdenum 95.94 $[Kr]4d^5 5s$ 7.0924	43 $^6S_{5/2}$ **Tc** Technetium (98) $[Kr]4d^5 5s^2$ 7.28	44 $^5F_5$ **Ru** Ruthenium 101.07 $[Kr]4d^7 5s$ 7.3605	45 $^4F_{9/2}$ **Rh** Rhodium 102.90550 $[Kr]4d^8 5s$ 7.4589	46 $^1S_0$ **Pd** Palladium 106.42 $[Kr]4d^{10}$ 8.3369	47 $^2S_{1/2}$ **Ag** Silver 107.8682 $[Kr]4d^{10} 5s$ 7.5762	48 $^1S_0$ **Cd** Cadmium 112.411 $[Kr]4d^{10} 5s^2$ 8.9938	49 $^2P^o_{1/2}$ **In** Indium 114.818 $[Kr]4d^{10} 5s^2 5p$ 5.7864	50 $^3P_0$ **Sn** Tin 118.710 $[Kr]4d^{10} 5s^2 5p^2$ 7.3439	51 $^4S^o_{3/2}$ **Sb** Antimony 121.760 $[Kr]4d^{10} 5s^2 5p^3$ 8.6084	52 $^3P_2$ **Te** Tellurium 127.60 $[Kr]4d^{10} 5s^2 5p^4$ 9.0096	53 $^2P^o_{3/2}$ **I** Iodine 126.90447 $[Kr]4d^{10} 5s^2 5p^5$ 10.4513	54 $^1S_0$ **Xe** Xenon 131.293 $[Kr]4d^{10} 5s^2 5p^6$ 12.1298
6	55 $^2S_{1/2}$ **Cs** Cesium 132.90545 [Xe]6s 3.8939	56 $^1S_0$ **Ba** Barium 137.327 $[Xe]6s^2$ 5.2117		72 $^3F_2$ **Hf** Hafnium 178.49 $[Xe]4f^{14} 5d^2 6s^2$ 6.8251	73 $^4F_{3/2}$ **Ta** Tantalum 180.9479 $[Xe]4f^{14} 5d^3 6s^2$ 7.5496	74 $^5D_0$ **W** Tungsten 183.84 $[Xe]4f^{14} 5d^4 6s^2$ 7.8640	75 $^6S_{5/2}$ **Re** Rhenium 186.207 $[Xe]4f^{14} 5d^5 6s^2$ 7.8335	76 $^5D_4$ **Os** Osmium 190.23 $[Xe]4f^{14} 5d^6 6s^2$ 8.4382	77 $^4F_{9/2}$ **Ir** Iridium 192.217 $[Xe]4f^{14} 5d^7 6s^2$ 8.9670	78 $^3D_3$ **Pt** Platinum 195.078 $[Xe]4f^{14} 5d^9 6s$ 8.9588	79 $^2S_{1/2}$ **Au** Gold 196.96655 $[Xe]4f^{14} 5d^{10} 6s$ 9.2255	80 $^1S_0$ **Hg** Mercury 200.59 $[Xe]4f^{14} 5d^{10} 6s^2$ 10.4375	81 $^2P^o_{1/2}$ **Tl** Thallium 204.3833 [Hg]6p 6.1082	82 $^3P_0$ **Pb** Lead 207.2 $[Hg]6p^2$ 7.4167	83 $^4S^o_{3/2}$ **Bi** Bismuth 208.98038 $[Hg]6p^3$ 7.2855	84 $^3P_2$ **Po** Polonium (209) $[Hg]6p^4$ 8.414	85 $^2P^o_{3/2}$ **At** Astatine (210) $[Hg]6p^5$	86 $^1S_0$ **Rn** Radon (222) $[Hg]6p^6$ 10.7485
7	87 $^2S_{1/2}$ **Fr** Francium (223) [Rn]7s 4.0727	88 $^1S_0$ **Ra** Radium (226) $[Rn]7s^2$ 5.2784		104 $^3F_2$? **Rf** Rutherfordium (261) $[Rn]5f^{14} 6d^2 7s^2$? 6.0 ?	105 **Db** Dubnium (262)	106 **Sg** Seaborgium (266)	107 **Bh** Bohrium (264)	108 **Hs** Hassium (277)	109 **Mt** Meitnerium (268)	110 **Uun** Ununnilium (281)	111 **Uuu** Unununium (272)	112 **Uub** Ununbium (285)		114 **Uuq** Ununquadium (289)		116 **Uuh** Ununhexium (292)		

Lanthanides	57 $^2D_{3/2}$ **La** Lanthanum 138.9055 $[Xe]5d6s^2$ 5.5769	58 $^1G^o_4$ **Ce** Cerium 140.116 $[Xe]4f5d6s^2$ 5.5387	59 $^4I^o_{9/2}$ **Pr** Praseodymium 140.90765 $[Xe]4f^3 6s^2$ 5.473	60 $^5I_4$ **Nd** Neodymium 144.24 $[Xe]4f^4 6s^2$ 5.5250	61 $^6H^o_{5/2}$ **Pm** Promethium (145) $[Xe]4f^5 6s^2$ 5.582	62 $^7F_0$ **Sm** Samarium 150.36 $[Xe]4f^6 6s^2$ 5.6437	63 $^8S^o_{7/2}$ **Eu** Europium 151.964 $[Xe]4f^7 6s^2$ 5.6704	64 $^9D^o_2$ **Gd** Gadolinium 157.25 $[Xe]4f^7 5d6s^2$ 6.1498	65 $^6H^o_{15/2}$ **Tb** Terbium 158.92534 $[Xe]4f^9 6s^2$ 5.8638	66 $^5I_8$ **Dy** Dysprosium 162.500 $[Xe]4f^{10} 6s^2$ 5.9389	67 $^4I^o_{15/2}$ **Ho** Holmium 164.93032 $[Xe]4f^{11} 6s^2$ 6.0215	68 $^3H_6$ **Er** Erbium 167.259 $[Xe]4f^{12} 6s^2$ 6.1077	69 $^2F^o_{7/2}$ **Tm** Thulium 168.93421 $[Xe]4f^{13} 6s^2$ 6.1843	70 $^1S_0$ **Yb** Ytterbium 173.04 $[Xe]4f^{14} 6s^2$ 6.2542	71 $^2D_{3/2}$ **Lu** Lutetium 174.967 $[Xe]4f^{14} 5d6s^2$ 5.4259
Actinides	89 $^2D_{3/2}$ **Ac** Actinium (227) $[Rn]6d^2 7s^2$ 5.17	90 $^3F_2$ **Th** Thorium 232.0381 $[Rn]6d^2 7s^2$ 6.3067	91 $^4K_{11/2}$ **Pa** Protactinium 231.03588 $[Rn]5f^2 6d^1 7s^2$ 5.89	92 $^5L_6$ **U** Uranium 238.02891 $[Rn]5f^3 6d^1 7s^2$ 6.1941	93 $^6L_{11/2}$ **Np** Neptunium (237) $[Rn]5f^4 6d^1 7s^2$ 6.2657	94 $^7F_0$ **Pu** Plutonium (244) $[Rn]5f^6 7s^2$ 6.0260	95 $^8S^o_{7/2}$ **Am** Americium (243) $[Rn]5f^7 7s^2$ 5.9738	96 $^9D^o_2$ **Cm** Curium (247) $[Rn]5f^7 6d^1 7s^2$ 5.9914	97 $^6H^o_{15/2}$ **Bk** Berkelium (247) $[Rn]5f^9 7s^2$ 6.1979	98 $^5I_8$ **Cf** Californium (251) $[Rn]5f^{10} 7s^2$ 6.2817	99 $^4I^o_{15/2}$ **Es** Einsteinium (252) $[Rn]5f^{11} 7s^2$ 6.42	100 $^3H_6$ **Fm** Fermium (257) $[Rn]5f^{12} 7s^2$ 6.50	101 $^2F^o_{7/2}$ **Md** Mendelevium (258) $[Rn]5f^{13} 7s^2$ 6.58	102 $^1S_0$ **No** Nobelium (259) $[Rn]5f^{14} 7s^2$ 6.65	103 $^2P^o_{1/2}$? **Lr** Lawrencium (262) $[Rn]5f^{14} 7s^2 7p$? 4.9 ?

Atomic Number — Ground-state Level
Symbol — Name — Atomic Weight† — Ground-state Configuration — Ionization Energy (eV)

58 $^1G^o_4$
Ce
Cerium
140.116
$[Xe]4f5d6s^2$
5.5387

†Based upon ^{12}C. () indicates the mass number of the most stable isotope.

For a description of the data, visit physics.nist.gov/data

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The Periodic Table (See Shankar pp.369-371, Griffiths sect. 5.2.2)

Understanding the periodic table is one fo the triumphs of QM. Recall that for hydrogen, the electron energy eigenstates are $|n,l,m\rangle$, where

$$n=1,2,3,\ldots \qquad l=0,1,\ldots,n-1 \qquad m=-l,\ \ldots,0,\ldots,l$$

n=principal quantum number, l=orbital quantum number, m=azimuthal (or magnetic) quantum number. At a given energy-level n, there are n^2 degenerate states.

Note too that since the electron is a spin-1/2 fermion, it can be in a spin-up or spin-down state of S_z. So the electron's state can be further specified by its spin quantum number $m_s = +1/2$ or $-1/2$.

Hence, the degeneracy at energy level n, including electron spin, is $2n^2$.

Spectroscopic notation: $l=0 \rightarrow$ s, $l=1 \rightarrow$p, $l=2 \rightarrow$d, $l=3 \rightarrow$ f, …

(So, for example, a 2p state refers to the state n=2, l=1.) Thus, the eigenstates (i.e. orbitals) for the electron are

1s, 2s, 2p, 3s, 3p, 3d, ….

Understanding Multi-electron atoms

The basic picture follows from some simple considerations/approximations

1) Crudest approximation: ignore all electron-electron interactions! So each electron is in one of the hydrogenic (i.e., single-electron) eigenstates (called "orbitals")

2) Pauli exclusion principle: no two electrons can occupy the same exact state

3) Electrons fill orbitals in order of increasing energy

4) Electron-electron interactions break the degeneracy in l of hydrogen: For a given n, states with higher l values tend to have higher energy (since higher l means more angular momentum, and such an electron tends to be farther from the nucleus and hence the inner electrons tend to "shield" the nucleus.

5) States with filled shells (i.e., n-levels) or filled subshells (i.e., subshells) tend to be chemically inert, since the total electric charge configuration is spherically symmetric, so they shield their nucleus effectively, and hence there is little electron affinity for electrons in other atoms.

With this in mind, we can now construct the expected ground states of various elements …

Element	1s	2s	2p	2p	2p	Electron configuration
H						$(1s)^1$
He						$(1s)^2$
Li						$(1s)^2(2s)^1$
Be						$(1s)^2(2s)^2$
B						$(1s)^2(2s)^2(2p)^1$
C						$(1s)^2(2s)^2(2p)^2$
N						$(1s)^2(2s)^2(2p)^3$
O						$(1s)^2(2s)^2(2p)^4$
F						$(1s)^2(2s)^2(2p)^5$
Ne						$(1s)^2(2s)^2(2p)^6$

Notice that He, Ne, Ar, Kr, ... making up the last column of the periodic table tend to be chemically inert. Elements in the first column, such as Li, Na, … have one "extra" electron, so to speak. This extra electron "sees" a net charge of only +e when it "looks inward", since the 10 inner electrons effectively "screen" much of the +11e nucleus – i.e., the outer electron in Na is only loosely bound to the atom. Thus, Na is fairly willing to give up this loosely bound "valence" electron to other atoms. Elements in the column next to the noble gas column, such as F, Cl, …"want" to receive an extra electron. So Na and F make a good match: Na will donate an electron to F, in which case both atoms are ionized, and thus held together by an "ionic bond."

As we continue along the periodic table, some of our preceding rules must be modified. For example, after argon Ar= $(Ne)(3s)^2(3p)^6$ comes potassium K =(Ar)(4s). Notice that we would have expected potassium's 19^{th} electron to go into the 3d state, not the 4s state. Why didn't it? Because the growth in energy due to the increase in l is larger than the increase in energy from n=3 to n=4, so it is energetically favorable for the extra electron to go into the 4s state!

Addition of Angular Momentum

Reading: Shankar chapt. 15 and Griffiths 4.4.3

We found that the angular-momentum state of a particle (either orbital or spin) could be represented by |j,m>, where j, m are "good quantum numbers" associated with the operators $\hat{J}^2$, $\hat{J}_z$:

$$\hat{J}^2 |j,m\rangle = \hbar^2 j(j+1) |j,m\rangle$$

$$\hat{J}_z |j,m\rangle = \hbar m |j,m\rangle$$

Here, "good" means that these numbers can be simultaneously specified, since the two operators commute. And of course we also determined commutation relations involving other related operators, including $\hat{J}_x$ $\hat{J}_y$, $\hat{J}_z$ $\hat{J}^2$, $\hat{J}_+$, $\hat{J}_-$.

e.g. $[\hat{J}_x, \hat{J}_y] = i\hbar \hat{J}_z$, etc.

If we have either

a) 2 (or more) distinct particles, each with its own angular momentum, such as in a multi-electron atom

b) A single particle that has both orbital and spin angular momentum, such as the electron of a hydrogen atom

Then we can ask questions about what the <u>total angular momentum</u> of the *system* is.

<u>Preliminaries</u>

Start with 2 angular momenta $\vec{J}_1, \vec{J}_2$ belonging to different subspaces (i.e., assume they commute):

$$[J_{1x}, J_{1y}] = i\hbar J_{1z}, \quad [J_{1y}, J_{1z}] = i\hbar J_{1x}, \quad [J_{1z}, J_{1x}] = i\hbar J_{1y}$$

$$[J_{2x}, J_{2y}] = i\hbar J_{2z}, \quad [J_{2y}, J_{2z}] = i\hbar J_{2x}, \quad [J_{2z}, J_{2x}] = i\hbar J_{2y}$$

$$[J_{1j}, J_{2k}] = 0 \qquad j = x, y, z, \quad k = x, y, z$$

The state of the composite system is given by

$$|j_1, m_1\rangle \otimes |j_2, m_2\rangle$$

(equivalent notation: $|j_1 m_1; j_2, m_2\rangle$ or: $|j_1, m_1\rangle|j_2, m_2\rangle$)

In this *uncoupled representation*, the system is specified by 4 quantum numbers, j_1, m_1, j_2, m_2. -- i.e., the operators $J_1^2, J_{1z}, J_2^2, J_{2z}$ form a complete set of commuting observables!

(Note: the dimensionality of the composite system is just the product of the dimensionality of the two subspaces).

The above representation is a perfectly good way of expressing the angular momentum state of the composite system. We now look at an alternative means of doing this which proves especially useful.

Total angular momentum

Define the total angular momentum $\vec{J} = \vec{J}_1 + \vec{J}_2$ ← I've dropped the hats on the operators

The magnitude and z-component of the total angular momentum for the composite system is described by operators

$$J^2 \equiv (\vec{J}_1 + \vec{J}_2)^2 = J_1^2 + J_2^2 + 2\vec{J}_1 \cdot \vec{J}_2$$

$$J_z \equiv J_{1z} + J_{2z}$$

Do these operators commute with one another? --YES

(Stop and verify this for yourself!)

So these operators share a common set of eigenvectors, and thus they provide us with two good quantum numbers. We'll call these j and m, and denote the eigenstate |j,m>. Since the total angular momentum is still just an angular momentum, by earlier arguments we have

$$J^2 |j,m\rangle = \hbar^2 j(j+1) |j,m\rangle \quad ; \quad J_z |j,m\rangle = \hbar m |j,m\rangle$$

where $m = -j, -j+1, \ldots 0, \ldots, j-1, j$ $\quad$ (Also, $[J_x, J_y] = i\hbar J_z$, etc.)

But wait! In the uncoupled representation, the angular momentum of the composite system is specified by 4 good quantum numbers. But so far, in terms of the total angular momentum, we have only found 2 good quantum numbers: j, associated with the magnitude of the total angular momentum, and m, associated with the z-component of the total angular momentum.

We'll need to hunt around for (two) additional operators that commute with one another and with $\vec{J}^2, J_z$.

I'll spare you the search: $\vec{J}^2, J_z, \vec{J}_1^2, \vec{J}_2^2$ form a complete set of commuting observables!

Let's do a quick, partial verification of this.

$$\begin{aligned}
[\vec{J}_1^2, \vec{J}^2] &= [\vec{J}_1^2, \vec{J}_1^2 + \vec{J}_2^2 + 2\vec{J}_1 \cdot \vec{J}_2] \\
&= 2[\vec{J}_1^2, \vec{J}_1 \cdot \vec{J}_2] \\
&= 2[\vec{J}_1^2, \vec{J}_1] \cdot \vec{J}_2 \\
&= 0
\end{aligned}$$

$$[J_1^2, J_z] = [J_1^2, J_{1z} + J_{2z}]$$
$$= [J_1^2, J_{1z}]$$
$$= 0$$

(Verify for yourself, for example, that J^2 doesn't commute with J_{1z} or with J_{2z})

We'll call the representation in which J^2, J_z, J_1^2, J_2^2 are specified the *coupled representation*, and denote the eigenstates by $|j, m, j_1, j_2\rangle$.

In the coupled representation, we have the obvious (or at least plausible) relations:

$$J^2 |j\ m\ j_1\ j_2\rangle = \hbar^2 j(j+1) |j\ m\ j_1\ j_2\rangle$$
$$J_z |j\ m\ j_1\ j_2\rangle = \hbar m |j\ m\ j_1\ j_2\rangle$$
$$J_1^2 |j\ m\ j_1\ j_2\rangle = \hbar^2 j_1(j_1+1) |j\ m\ j_1\ j_2\rangle$$
$$J_2^2 |j\ m\ j_1\ j_2\rangle = \hbar^2 j_2(j_2+1) |j\ m\ j_1\ j_2\rangle$$

Relation between representations

So we have two perfectly good bases for describing the angular momentum of a composite system:

$$|j_1, m_1\rangle |j_2, m_2\rangle \quad \text{and} \quad |j, m; j_1, j_2\rangle$$

What's the relation between the two? Let's start with the quantum numbers themselves.

$$\text{Since} \quad J_z\, |j_1, m_1\rangle |j_2, m_2\rangle \equiv (J_{1z} + J_{2z})\, |j_1, m_1\rangle |j_2, m_2\rangle$$

$$= \hbar (m_1 + m_2)\, |j_1, m_1\rangle |j_2, m_2\rangle$$

$$\Rightarrow \quad m = m_1 + m_2$$

Now, since the max value of m_1 is j_1, and since the max value of m_2 is j_2, it follows that $m_{max}=j_1+j_2$. But we also know that m ranges from –j, …, j. Hence we can conclude that $\mathbf{j_{max}=j_1+j_2}$. (Perhaps this isn't surprising: classically, the magnitude of the total angular momentum of a composite system can't exceed that of its individual components.

Reasoning classically, we might also anticipate that there is a minimum value of j for the composite system, given by the difference $|j_1-j_2|$ (corresponding to when the angular momentum of the individual components of the system point in opposite directions). This is indeed the case, as we now show using a counting argument:

For a given j_1, j_2, there are a total of $(2j_1+1)(2j_2+1)$ independent basis vectors of the form $|j_1,m_1\rangle\,|j_2,m_2\rangle$.

This must be the same total as for the $|j,m, j_1,j_2\rangle$ basis (with j_1, j_2 fixed as before). Now, for each j, there are (2j+1) possible m values.

So we demand that

$$\sum_{j_{min}}^{j_{max}=j_1+j_2}(2j+1) = (2j_1+1)(2j_2+1)$$

$$\Rightarrow \quad j_{min} = |j_1-j_2|$$

Summarizing,

$$m = m_1 + m_2$$

$$j = |j_1 - j_2|, \ldots, j_1 + j_2$$

Now let's compute the relationship between the basis vectors of the coupled and uncoupled representations:

$$|j\ m\ j_1\ j_2\rangle = \sum_{m_1+m_2=m} \sum C_{m_1 m_2} |j_1, m_1, j_2, m_2\rangle$$

where $C_{m_1 m_2} = \langle j_1, m_1, j_2, m_2 | j\ m\ j_1\ j_2 \rangle$

The coefficients $C_{m_1 m_2}$ are called the *Clebsch-Gordan* coefficients.

Their interpretation is straightforward: $|C_{m_1 m_2}|^2$ gives the probability that, for a specified j and m, a measurement of j_{1z} will yield the value m_1 <u>and</u> a measurement of j_{2z} will yield the value m_2 .

Calculation of the Clebsch-Gordan coefficients can be done by appropriate application of the raising/lowering operators J_+,J_- (though we note that these calculations tend to be tedious, so look-up tables exist to assist you).

[Note: The standard phase convention used when defining basis vectors $|j,m,j_1,j_2\rangle$ is such that all Clebsch-Gordan coefficients are purely real, and that the projection $\langle j_1, m_1=j_1; j_2, m_2=j-j_1 \mid j,m,j_1,j_2\rangle$ is real.]

Here's an example calculation:

What does the state $|1,-1,1,1\rangle$ look like in the uncoupled representation?

Solution : $j_1 = 1 \longrightarrow m_1 = 1,0,-1$

$j_2 = 1 \longrightarrow m_2 = 1,0,-1$

But $m = m_1 + m_2 \longrightarrow -1 = m_1 + m_2 \longrightarrow (m_1=0, m_2=-1)$ or $(m_1=-1, m_2=0)$

$$\Rightarrow |1,-1,1,1\rangle = C_{0,-1}\,|1,0\rangle|1,-1\rangle + C_{-1,0}\,|1,-1\rangle|1,0\rangle$$

Hit both sides w/ $J_- \equiv J_{1-} + J_{2-}$

LHS: $J_- |1,-1,1,i\rangle = 0$ (since for $j=1$, m can't go below -1)

RHS: $(J_{1-} + J_{2-})\left[C_{0,-1} |1,0\rangle|1,-1\rangle + C_{-1,0} |1,-1\rangle|1,0\rangle \right]$

$= C_{0,-1} |1,-1\rangle|1,-1\rangle + C_{-1,0} |1,-1\rangle|1,-1\rangle$

Setting LHS = RHS $\Rightarrow$ $0 = C_{0,-1} + C_{-1,0}$

$\longrightarrow C_{0,-1} = -C_{-1,0}$. Normalization of $|1,-1,1,1\rangle$

gives $C_{0,-1} = \frac{1}{\sqrt{2}}$

$$|1,-1,1,1\rangle = \frac{1}{\sqrt{2}} |1,0\rangle|1,-1\rangle - \frac{1}{\sqrt{2}} |1,-1\rangle|1,0\rangle$$

■

It's easy to find the Clebsch-Gordan coefficients in two limiting cases:

1) $|j_1+j_2, j_1+j_2, j_1, j_2\rangle = 1 \cdot |j_1, j_1\rangle |j_2, j_2\rangle$

2) $|j_1+j_2, -(j_1+j_2), j_1, j_2\rangle = 1 \cdot |j_1, -j_1\rangle |j_2, -j_2\rangle$

If you're interested in a general way of calculating Clebsch-Gordan coefficients, the following (recursion) relation proves useful:

Consider: $\langle \underbrace{j_1, m_1, j_2, m_2}_{\text{uncoupled rep.}} | J_\pm | \underbrace{j, m, j_1, j_2}_{\text{coupled}} \rangle$.

Evaluate in 2 different ways:

A) allow $J_\pm$ to act to the right.

$$\Rightarrow \hbar \sqrt{(j \mp m)(j \pm m + 1)} \langle j_1, m_1, j_2, m_2 | j, m \pm 1, j_1, j_2 \rangle$$

B) allow $J_\pm \equiv J_{1\pm} + J_{2\pm}$ to act to the left.

$$\Rightarrow \hbar \sqrt{(j_1 \pm m_1)(j_1 \mp m_1 + 1)} \langle j_1, m_1 \mp 1, j_2, m_2 | j, m, j_1, j_2 \rangle + \hbar \sqrt{(j_2 \pm m_2)(j_2 \mp m_2 + 1)} \langle j_1, m_1, j_2, m_2 \mp 1 | j, m, j_1, j_2 \rangle$$

Equating these two expressions leads to a useful relation that allows one to (recursively) generate all Clebsch-Gordan coefficients (provided one uses the orthogonality conditions as well).

Example 1: The allowed (m_1,m_2) and (j,m) values if $j_1=1$ and $j_2=3/2$

m_1	m_2	m	j
1	3/2	5/2	5/2
0	3/2	3/2	5/2, 3/2
1	1/2	3/2	5/2, 3/2
-1	3/2	1/2	5/2, 3/2, 1/2
0	1/2	1/2	5/2, 3/2, 1/2
1	-1/2	1/2	5/2, 3/2, 1/2
-1	1/2	-1/2	5/2, 3/2, 1/2
0	-1/2	-1/2	5/2, 3/2, 1/2
1	-3/2	-1/2	5/2, 3/2, 1/2
-1	-1/2	-3/2	5/2, 3/2
0	-3/2	-3/2	5/2, 3/2
-1	-3/2	-5/2	5/2

Notes:

a) There are 12 distinct combinations of (m_1,m_2), and 12 distinct combo's of (j,m)

b) Table is organized by decreasing m values.

Example 2: Two spin ½ particles

Total spin : $S = 1$ or $S = 0$ $\quad (s_1 = \frac{1}{2},\ s_2 = \frac{1}{2})$

z-component of Total Spin : $m_s = m_{s1} + m_{s2} \Rightarrow m_s = 1, 0, -1$

(m_{s1}: $\uparrow$ $\pm 1/2$; m_{s2}: $\uparrow$ $\pm 1/2$)

If $S = 1 \longrightarrow m_s = 1, 0, -1$ (Triplet state)

$S = 0 \longrightarrow m_s = 0$ (Singlet state)

triplet:

$$|1, 1, \tfrac{1}{2}, \tfrac{1}{2}\rangle = |\tfrac{1}{2}, \tfrac{1}{2}\rangle|\tfrac{1}{2}, \tfrac{1}{2}\rangle$$

$$|1, 0, \tfrac{1}{2}, \tfrac{1}{2}\rangle = \frac{1}{\sqrt{2}}\left[|\tfrac{1}{2}\ \tfrac{1}{2}\rangle|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle + |\tfrac{1}{2}\ -\tfrac{1}{2}\rangle|\tfrac{1}{2}\ \tfrac{1}{2}\rangle\right]$$

$$|1, -1, \tfrac{1}{2}, \tfrac{1}{2}\rangle = |\tfrac{1}{2}, -\tfrac{1}{2}\rangle|\tfrac{1}{2}, -\tfrac{1}{2}\rangle$$

singlet:

$$|0, 0, \tfrac{1}{2}, \tfrac{1}{2}\rangle = \frac{1}{\sqrt{2}}\left[|\tfrac{1}{2}, \tfrac{1}{2}\rangle|\tfrac{1}{2}\ -\tfrac{1}{2}\rangle - |\tfrac{1}{2}, -\tfrac{1}{2}\rangle|\tfrac{1}{2}, \tfrac{1}{2}\rangle\right]$$

Example 3: Angular momentum of two p electrons (i.e., $j_1=1$ and $j_2=1$).

$$|j\, m\, j_1, j_2\rangle \equiv \sum C_{m_1 m_2}\, |j_1\, m_1\rangle |j_2\, m_2\rangle$$

①	$\|2\,2\,1\,1\rangle = \|1\,1\rangle\,\|1\,1\rangle$
②	$\|2\,1\,1\,1\rangle = \frac{1}{\sqrt{2}}\|1\,1\rangle\|1\,0\rangle + \frac{1}{\sqrt{2}}\|1\,0\rangle\|1\,1\rangle$
③	$\|2\,0\,1\,1\rangle = \frac{1}{\sqrt{6}}\|1\,1\rangle\|1\,-1\rangle + \sqrt{\frac{2}{3}}\|1\,0\rangle\|1\,0\rangle + \frac{1}{\sqrt{6}}\|1\,-1\rangle\|1\,1\rangle$
④	$\|2\,-1\,1\,1\rangle = \frac{1}{\sqrt{2}}\|1\,0\rangle\|1\,-1\rangle + \frac{1}{\sqrt{2}}\|1\,-1\rangle\|1\,0\rangle$
⑤	$\|2\,-2\,1\,1\rangle = \|1\,-1\rangle\,\|1\,-1\rangle$
⑥	$\|1\,1\,1\,1\rangle = \frac{1}{\sqrt{2}}\|1\,1\rangle\|1\,0\rangle - \frac{1}{\sqrt{2}}\|1\,0\rangle\|1\,1\rangle$
⑦	$\|1\,0\,1\,1\rangle = \frac{1}{\sqrt{2}}\|1\,1\rangle\|1\,-1\rangle - \frac{1}{\sqrt{2}}\|1\,-1\rangle\|1\,1\rangle$
⑧	$\|1\,-1\,1\,1\rangle = \frac{1}{\sqrt{2}}\|1\,0\rangle\|1\,-1\rangle - \frac{1}{\sqrt{2}}\|1\,-1\rangle\|1\,0\rangle$
⑨	$\|0\,0\,1\,1\rangle = \frac{1}{\sqrt{3}}\|1\,1\rangle\|1\,-1\rangle - \frac{1}{\sqrt{3}}\|1\,0\rangle\|1\,0\rangle + \frac{1}{\sqrt{3}}\|1\,-1\rangle\|1\,1\rangle$

To show this, will need $J_- |j\ m\ j_1 j_2\rangle = \hbar \sqrt{(j+m)(j-m+1)}\, |j\ m-1\ j_1 j_2\rangle$

plus orthogonality relations (plus phase choice) :

① follows because there's only one choice!

To get ②, apply $J_- = J_{1-} + J_{2-}$ to ① :

$$J_- |2\,2\,i\,i\rangle = (J_{1-} + J_{2-}) |i\,i\rangle |i\,i\rangle$$

$$\Rightarrow \quad \hbar |2\,1\,i\,i\rangle = \sqrt{2}\,\hbar \left[|i\,i\rangle |i\,0\rangle + |i\,0\rangle |i\,i\rangle \right]$$

To get ③ apply $J_- = J_{1-} + J_{2-}$ to both sides of ②. Keep on doing this to get ④ and ⑤.

To get ⑥ : we know $|1\,1\,i\,i\rangle = a|i\,i\rangle|i\,0\rangle + b|i\,0\rangle|i\,i\rangle$

but $\langle 1111|1111\rangle = 1 \longrightarrow a^2 + b^2 = 1$

Also, $\langle 2111|1111\rangle = 0 \longrightarrow \frac{a}{\sqrt{2}} + \frac{b}{\sqrt{2}} = 0$

$\Rightarrow a = \pm\frac{1}{\sqrt{2}}, b = \mp\frac{1}{\sqrt{2}}$. Phase convention says

$\langle j_1, m_1 = j_1, j_2, m_2 = j - j_1 | j j, j_1, j_2\rangle$ = positive

$\Rightarrow a = \frac{1}{\sqrt{2}}, b = -\frac{1}{\sqrt{2}}$

Apply $J_- = J_{1-} + J_{2-}$ to both sides of ⑥ to get ⑦. Apply this again to ⑦ to get ⑧.

To get ⑨: we know $|00,11\rangle = a|11\rangle|1-1\rangle + b|10\rangle|10\rangle + c|1-1\rangle|11\rangle$

demand $\langle 0011|0011\rangle = 1 \longrightarrow a^2 + b^2 + c^2 = 1$

demand $\langle 2011|0011\rangle = 0 \longrightarrow \frac{a}{\sqrt{6}} + \frac{2b}{\sqrt{6}} + \frac{c}{\sqrt{6}} = 0$

demand $\langle 1011|0011\rangle = 0 \longrightarrow \frac{a}{\sqrt{2}} - \frac{c}{\sqrt{2}} = 0$

phase convention $\Rightarrow$ a is positive

$\Rightarrow \quad a = \frac{1}{\sqrt{3}}, \quad b = -\frac{1}{\sqrt{3}}, \quad c = \frac{1}{\sqrt{3}}$!