Solution Set 10

First we are supposed to show that the listed wave functions have the proper boundary conditions; that is, that they vanish at the boundaries. Plugging in the boundary values, we see that at $x = \pm a$ yields a factor of $w_l\left(\pm\frac{1}{2}\pi l\right)$. Recalling that cosine vanishes at odd multiples of $\frac{1}{2}\pi$, while sine vanishes at even multiples, we conclude that $\psi_{lmn}\left(\pm a, y, z\right) = 0$. Similarly, $y = \pm a$ and $z = \pm b$ yield factors of $w_m\left(\pm\frac{1}{2}\pi m\right)$ and $w_n\left(\pm\frac{1}{2}\pi n\right)$, both of which vanish, so $\psi_{lmn}\left(x, \pm a, z\right) = \psi_{lmn}\left(x, y, \pm b\right) = 0$.

First we need to figure out the effect of the various types of operations on the various wave functions. For example, C_4^2 reverses both *x* and *y*, and therefore

$$C_4^2 \psi_{lmn} = \left(-1\right)^{l+m} \psi_{lmn}$$

For representations A_1, A_2, B_1, and B_2, this tells us that we only build these irreps out of wave functions where $l + m$ is even.

Similarly, C_2' can either reverse *x* and *z*, or *y* and *z*. For example, one of the elements has the effect

$$C_{2a}' \psi_{lmn} = \left(-1\right)^{l+n} \psi_{lmn}$$

This tells you that for A_1 and B_1, $l+n$ will be even, while for A_2 and B_2, they will be odd.

To finish off these four cases, consider C_4, one element of which exchanges *x* and *y* while changing the sign of one of them, so that

$$C_4 \psi_{lmn} = \left(-1\right)^{l+1} \psi_{mln}$$

If we set $l = m$, for example, we can get the *A*'s by picking *l* odd, and the *B*'s by picking *l* even. This is sufficient to determine the following four categorizations:

A_1: ψ_{111} A_2: ψ_{112} B_1: ψ_{222} B_2: ψ_{221}

This leaves only the case when $l + m$ is odd, in which case C_4^2 changes the sign of everything, assuring that we are in the representation *E*. We therefore need pairs of wave functions that will rotate into each other under some of the elements. The lowest energy answer is obviously ψ_{211} and ψ_{121}, which clearly will get converted into each other by C_4 rotations.

$$E: \ \left\{\psi_{211}, \psi_{121}\right\}$$