Physics 745 - Group Theory

Solution Set 12

Due Monday, February 16

1. Diamond is a version of carbon. The position of the carbon atoms takes the form

$$\mathbf{r} = d\left(n_1 + x\right)\hat{\mathbf{x}} + d\left(n_2 + y\right)\hat{\mathbf{y}} + d\left(n_3 + z\right)\hat{\mathbf{z}}$$

where *d* = 356.683 pm, $\left(n_1, n_2, n_3\right)$ are arbitrary integers, and $\left(x, y, z\right)$ takes on the following eight values:

$$\left(x,y,z\right) \in \left\{\left(0,0,0\right),\left(\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}\right),\left(0,\tfrac{1}{2},\tfrac{1}{2}\right),\left(\tfrac{1}{2},\tfrac{1}{2},0\right),\left(\tfrac{1}{2},0,\tfrac{1}{2}\right),\left(\tfrac{1}{4},\tfrac{3}{4},\tfrac{3}{4}\right),\left(\tfrac{3}{4},\tfrac{1}{4},\tfrac{3}{4}\right),\left(\tfrac{3}{4},\tfrac{3}{4},\tfrac{1}{4}\right)\right\}$$

Thus there are eight carbon atoms per cell of size d^3.

(a) For what values of $\left(x, y, z\right)$ will $\mathbf{T} = dx\hat{\mathbf{x}} + dy\hat{\mathbf{y}} + dz\hat{\mathbf{z}}$ be a translation vector; *i.e.*, if there is a carbon atom at r, there will always be a carbon atom at $\mathbf{r}+\mathbf{T}$? To make your answer finite, only include values with $0 \le x, y, z < 1$.

If **T** is a translation vector, we should be able to add it to the position of the first carbon atom and we should get a new carbon atom. In particular, if we add it to the carbon at position (0,0,0), we should get another carbon. It follows that **T** must be one of the eight vectors listed above. So the answer is some subset of the list above.

Now, suppose we take any of the eight vectors listed above and add it to another vector, say $\left(\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}\right)$ The result, in the same order as above, is the vectors

$$\left(\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}\right),\left(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}\right),\left(\tfrac{1}{4},\tfrac{3}{4},\tfrac{3}{4}\right),\left(\tfrac{3}{4},\tfrac{3}{4},\tfrac{1}{4}\right),\left(\tfrac{3}{4},\tfrac{1}{4},\tfrac{3}{4}\right),\left(\tfrac{1}{2},1,1\right),\left(1,\tfrac{1}{2},1\right),\left(1,1,\tfrac{1}{2}\right)$$

Now, the first, third, fourth, and fifth of these are positions of carbon atoms. The other four are not. For example, $\left(\tfrac{1}{2},1,1\right)$ is the same as $\left(\tfrac{1}{2},0,0\right)$, which is not one of the carbon atoms. This means that **T** must be one of the four vectors that mapped to carbon atoms when we added them to $\left(\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}\right)$, so our choices are

$$\mathbf{T} \in \left\{d\left(0,0,0\right), d\left(0,\tfrac{1}{2},\tfrac{1}{2}\right), d\left(\tfrac{1}{2},\tfrac{1}{2},0\right), d\left(\tfrac{1}{2},0,\tfrac{1}{2}\right)\right\}$$

Obviously, the first one is an element of the translation group. To check the other three, add each of them to the locations of the original carbon atoms. The results are:

$$\left(0,\tfrac{1}{2},\tfrac{1}{2}\right): \quad \left(0,\tfrac{1}{2},\tfrac{1}{2}\right),\left(\tfrac{1}{4},\tfrac{3}{4},\tfrac{3}{4}\right),\left(0,1,1\right),\left(\tfrac{1}{2},1,\tfrac{1}{2}\right),\left(\tfrac{1}{2},\tfrac{1}{2},1\right),\left(\tfrac{1}{4},\tfrac{5}{4},\tfrac{5}{4}\right),\left(\tfrac{3}{4},\tfrac{3}{4},\tfrac{5}{4}\right),\left(\tfrac{3}{4},\tfrac{5}{4},\tfrac{3}{4}\right)$$
$$\left(\tfrac{1}{2},\tfrac{1}{2},0\right): \quad \left(\tfrac{1}{2},\tfrac{1}{2},0\right),\left(\tfrac{3}{4},\tfrac{3}{4},\tfrac{1}{4}\right),\left(\tfrac{1}{2},1,\tfrac{1}{2}\right),\left(1,1,0\right),\left(1,\tfrac{1}{2},\tfrac{1}{2}\right),\left(\tfrac{3}{4},\tfrac{5}{4},\tfrac{3}{4}\right),\left(\tfrac{5}{4},\tfrac{3}{4},\tfrac{5}{4}\right),\left(\tfrac{5}{4},\tfrac{5}{4},\tfrac{1}{4}\right)$$
$$\left(\tfrac{1}{2},0,\tfrac{1}{2}\right): \quad \left(\tfrac{1}{2},0,\tfrac{1}{2}\right),\left(\tfrac{3}{4},\tfrac{1}{4},\tfrac{3}{4}\right),\left(\tfrac{1}{2},\tfrac{1}{2},1\right),\left(1,\tfrac{1}{2},\tfrac{1}{2}\right),\left(1,0,1\right),\left(\tfrac{3}{4},\tfrac{3}{4},\tfrac{5}{4}\right),\left(\tfrac{5}{4},\tfrac{1}{4},\tfrac{5}{4}\right),\left(\tfrac{5}{4},\tfrac{3}{4},\tfrac{3}{4}\right)$$

Everyone of these corresponds exactly to one of the original positions of a carbon atom. This is obvious if we subtract one from any component exceeding one. So all four vectors **T** listed above are elements of the translation group.

(b) Find primitive vectors a, b and c such that *all* translation vectors take the form $\mathbf{T} = m_1\mathbf{a} + m_2\mathbf{b} + m_3\mathbf{c}$, where (m_1, m_2, m_3) are integers. Demonstrate it explicitly for those vectors you found in part (a) (which will probably be trivial), and also for the three vectors $d\hat{\mathbf{x}}$, $d\hat{\mathbf{y}}$ and $d\hat{\mathbf{z}}$.

A reasonable guess might be to choose the three vectors to correspond to the three non-zero elements of the translation group listed above, so we let

$$\mathbf{a} = \tfrac{1}{2}d\left(\hat{\mathbf{x}} + \hat{\mathbf{y}}\right)$$
$$\mathbf{b} = \tfrac{1}{2}d\left(\hat{\mathbf{x}} + \hat{\mathbf{z}}\right)$$
$$\mathbf{c} = \tfrac{1}{2}d\left(\hat{\mathbf{y}} + \hat{\mathbf{z}}\right)$$

It is trivial that these three vectors can be written in the form $\mathbf{T} = m_1\mathbf{a} + m_2\mathbf{b} + m_3\mathbf{c}$. As for the original basis vectors, it isn't hard to show that

$$d\hat{\mathbf{x}} = \mathbf{a} + \mathbf{b} - \mathbf{c}$$
$$d\hat{\mathbf{y}} = \mathbf{a} + \mathbf{c} - \mathbf{b}$$
$$d\hat{\mathbf{z}} = \mathbf{b} + \mathbf{c} - \mathbf{a}$$

This shows that **a**, **b** and **c** form a primitive basis for the translation group.

(c) What are the lengths of these vectors a, b, c and the angles between them, α, β, γ?

The lengths are obviously all the same, and so are the angles, so

$$a = b = c = \sqrt{\left(\tfrac{1}{2}d\right)^2 + \left(\tfrac{1}{2}d\right)^2} = \sqrt{\tfrac{1}{2}d^2} = d/\sqrt{2} = 252.213 \text{ pm},$$

$$\cos\gamma = \frac{\mathbf{a}\cdot\mathbf{b}}{ab} = \frac{\tfrac{1}{4}d^2}{\left(d/\sqrt{2}\right)^2} = \frac{1}{2}, \quad \alpha = \beta = \gamma = 60^\circ$$