Physics 745 - Group Theory

Solution Set 14

We use the general formula given by Dr. Holzwarth to find the scattering amplitude

$$S(\Delta\mathbf{k}) = \frac{(2\pi)^3}{\Omega}\sum_{\mathbf{G}}\delta^3(\Delta\mathbf{k}-\mathbf{G})\sum_a F_a(\Delta\mathbf{k})\sum_{\boldsymbol{\sigma}_a} e^{i\mathbf{G}\cdot\boldsymbol{\sigma}_a}$$

As inspired in class, we will ignore the delta function, and replace it by something like $\mathcal{I}(\mathbf{G})$. The volume in each case is easily worked out to be

$$\Omega = \left|(\mathbf{T}_1\times\mathbf{T}_2)\cdot\mathbf{T}_3\right| = \tfrac{1}{8}a^3\left|\left[(\hat{\mathbf{x}}+\hat{\mathbf{y}})\times(\hat{\mathbf{x}}+\hat{\mathbf{z}})\right]\cdot(\hat{\mathbf{y}}+\hat{\mathbf{z}})\right| = \tfrac{1}{8}a^3\left|\left[-\hat{\mathbf{y}}-\hat{\mathbf{z}}+\hat{\mathbf{x}}\right]\cdot(\hat{\mathbf{y}}+\hat{\mathbf{z}})\right| = \tfrac{1}{4}a^3$$

We now simply need to do the sums. We will always write $\mathbf{G} = m_1\mathbf{G}_1 + m_2\mathbf{G}_2 + m_3\mathbf{G}_3$, then we see that

$$\mathbf{G}\cdot\boldsymbol{\sigma}_{\text{Na}} = 0, \quad \mathbf{G}\cdot\boldsymbol{\sigma}_{\text{Cl}} = m_1\pi + m_2\pi + m_3\pi = \pi(m_1+m_2+m_3)$$

Substituting into our formulas, we then see that

$$S(\Delta\mathbf{k}) = 32\pi^3 a^{-3}\sum_{\mathbf{G}}\mathcal{I}(\mathbf{G})\left[F_{\text{Na}}(\Delta\mathbf{k})e^0 + F_{\text{Cl}}(\Delta\mathbf{k})e^{i\pi(m_1+m_2+m_3)}\right]$$
$$= 32\pi^3 a^{-3}\sum_{\mathbf{G}}\mathcal{I}(\mathbf{G})\left[F_{\text{Na}}(\Delta\mathbf{k}) + (-1)^{m_1+m_2+m_3}F_{\text{Cl}}(\Delta\mathbf{k})\right]$$

It is possible, but not helpful, to substitute the explicit form for these form factors. There is no reason to expect the sodium and chlorine contributions to cancel when $m_1+m_2+m_3$ is odd, though we might expect these peaks to be suppressed.

For diamond, we find

$$\mathbf{G}\cdot\boldsymbol{\sigma}_{\text{C1}} = -\tfrac{1}{4}\pi(m_1+m_2+m_3), \quad \mathbf{G}\cdot\boldsymbol{\sigma}_{\text{C2}} = \tfrac{1}{4}\pi(m_1+m_2+m_3)$$

This yields

$$S(\Delta\mathbf{k}) = 32\pi^3 a^{-3}\sum_{\mathbf{G}}\mathcal{I}(\mathbf{G})F_C(\Delta\mathbf{k})\left[e^{-i\pi(m_1+m_2+m_3)/4} + e^{i\pi(m_1+m_2+m_3)/4}\right]$$
$$= 64\pi^3 a^{-3}\sum_{\mathbf{G}}\mathcal{I}(\mathbf{G})F_C(\Delta\mathbf{k})\cos\left[\tfrac{1}{4}\pi(m_1+m_2+m_3)\right]$$

This vanishes whenever $m_1+m_2+m_3$ is singly even (*i.e.*, divisible by two but not four).