8.511 Theory of Solids I **Problem Set 2** **Due 8:00pm September 29, 2015**

1. Show that rotations about any axis that takes a Bravais lattice into itself must be either 1, 2, 3, 4 or 6 fold.

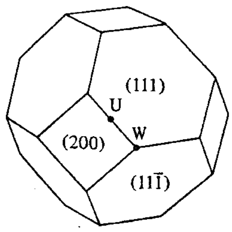

Figure 9.14
First Brillouin zone for a face-centered cubic crystal.

2. *Problem 3 from page 171 of Ashcroft & Mermin.* **Effect of Weak Periodic Potential at Places in *k*-Space where Bragg Planes Meet.** Consider the point W($\vec{k}_{\mathrm{W}} = (2\pi/a)(1, \frac{1}{2}, 0)$) in the Brillouin zone of the fcc structure shown (see Fig. 9.14). Here three Bragg planes ($(200), (111), (11\bar{1})$) meet, and accordingly the free electron energies

$$\begin{aligned}
\varepsilon_1^0 &= \frac{\hbar^2}{2m}k^2, \\
\varepsilon_2^0 &= \frac{\hbar^2}{2m}\left(\vec{k} - \frac{2\pi}{a}(1,1,1)\right)^2, \\
\varepsilon_3^0 &= \frac{\hbar^2}{2m}\left(\vec{k} - \frac{2\pi}{a}(1,1,\bar{1})\right)^2, \\
\varepsilon_4^0 &= \frac{\hbar^2}{2m}\left(\vec{k} - \frac{2\pi}{a}(2,0,0)\right)^2,
\end{aligned} \tag{1}$$

are degenerate when $\vec{k} = \vec{k}_{\mathrm{W}}$, and equal to $\varepsilon_{\mathrm{W}} = \hbar^2 \vec{k}_{\mathrm{W}}^2/2m$.

(a) Show that in a region of k space near W, the first-order energies are given by solutions to [1]

$$\begin{vmatrix}
\varepsilon_1^0 - \varepsilon & U_1 & U_1 & U_2 \\
U_1 & \varepsilon_2^0 - \varepsilon & U_2 & U_1 \\
U_1 & U_2 & \varepsilon_3^0 - \varepsilon & U_1 \\
U_2 & U_1 & U_1 & \varepsilon_4^0 - \varepsilon
\end{vmatrix} = 0$$

where $U_2 = U_{200}$, $U_1 = U_{111} = U11\bar{1}$, and that at W the roots are

$$\varepsilon = \varepsilon_{\mathrm{w}} - U_2 \quad \text{(twice)}, \quad \varepsilon = \varepsilon_{\mathrm{w}} + \mathrm{U}_2 \pm 2\mathrm{U}_1. \tag{2}$$

(b) Using a similar method, show that the energies at the point $U(\vec{k}_{\mathrm{U}} = (2\pi/a)(1, \frac{1}{4}, \frac{1}{4}))$ are

$$\varepsilon = \varepsilon_{\mathrm{U}} - U_2, \varepsilon = \varepsilon_{\mathrm{U}} + \frac{1}{2}U_2 \pm \frac{1}{2}(U_2^2 + 8U_1^2)^{1/2} \tag{3}$$

where $\varepsilon_{\mathrm{U}} = \hbar^2 \vec{k}_{\mathrm{U}}^2/2m$.

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[1] Assume that the periodic potential U has inversion symmetry so that the $U_{\vec{k}}$ are real.