8.511 Problem Set 2

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1 Problem 1

The notation below does not distinguish a vector from its endpoint. So if a vector starts from the origin o and ends at some lattice point u, I call this vector u.

In a Bravais lattice, a nonzero vector of the minimal length exists. Denote it by u, and let $d = |u|$. The rotation ρ (by an angle θ), whose axis does not necessarily pass through a lattice point, carries the origin o to some lattice point o'. Let $v = t_{-o'} \circ \rho(u)$. Then v has the same length as u (its start point is translated back to o). $u - v$ is also a lattice point. Its length is

$$\begin{aligned}|u - v|^2 &= |u|^2 + |v|^2 - 2|u||v|\cos\theta \\ &= 2d^2(1 - \cos\theta)\end{aligned}$$

Since u has the minimal length among all lattice points, $2d^2(1 - \cos\theta) \geqslant d^2$. This means $\theta \geqslant \frac{\pi}{3}$. As a result, 7- or more-fold rotations cannot exist.

The reason for 5-fold rotation to be forbidden is, let $w = t_{-o'} \circ \rho(v)$. Compared with u, w is rotated twice, so the angle between u and w is $\frac{4\pi}{5}$. Now consider $u + w$. Its length is given by

$$|u + w| = 2d\cos\frac{2\pi}{5} < d$$

which contradicts with the fact that u has minimal length. Therefore, 5-fold rotation cannot exist.

The rest rotations exist and there are examples of them. 1-fold rotation is trivial. 2- and 4- fold rotation exist in square lattices. 3- and 6- fold rotation exist in hexagonal lattices.

2 Problem 2

2.1 Part (a)

Let $\vec{k}_1 = \vec{k}_W$, $\vec{k}_2 = \vec{k}_W - \frac{2\pi}{a}(1,1,1)$, $\vec{k}_3 = \vec{k}_W - \frac{2\pi}{a}(1,1,-1)$ and $\vec{k}_4 = \vec{k}_W - \frac{2\pi}{a}(2,0,0)$. The four corresponding kinetic energies ε_i^0, $i = 1,2,3,4$ are degenerate and equal to ε_W. Their couplings are determined by

$$\begin{aligned}\vec{k}_1 - \vec{k}_2 &= \frac{2\pi}{a}(1,1,1) \to U_{111} \\ \vec{k}_1 - \vec{k}_3 &= \frac{2\pi}{a}(1,1,-1) \to U_{11\bar{1}} \\ \vec{k}_1 - \vec{k}_4 &= \frac{2\pi}{a}(2,0,0) \to U_{200} \\ \vec{k}_2 - \vec{k}_3 &= \frac{2\pi}{a}(0,0,-2) \to U_{00\bar{2}} \\ \vec{k}_2 - \vec{k}_4 &= \frac{2\pi}{a}(1,-1,-1) \to U_{1\bar{1}\bar{1}} \\ \vec{k}_3 - \vec{k}_4 &= \frac{2\pi}{a}(1,-1,1) \to U_{1\bar{1}1}\end{aligned}$$

According to symmetry, the Fourier components $U_{111} = U_{11\bar{1}} = U_{1\bar{1}1} = U_{\bar{1}11} = U_{1\bar{1}\bar{1}} = U_{\bar{1}1\bar{1}} = U_{\bar{1}\bar{1}1} = U_{\bar{1}\bar{1}\bar{1}} = U_1$, and $U_{200} = U_{020} = U_{002} = U_{\bar{2}00} = U_{0\bar{2}0} = U_{00\bar{2}} = U_2$. Then in the subspace spanned by the four plane waves, the Hamiltonian is

$$H = \begin{pmatrix} \varepsilon_1^0 & U_1 & U_1 & U_2 \\ U_1 & \varepsilon_2^0 & U_2 & U_1 \\ U_1 & U_2 & \varepsilon_3^0 & U_1 \\ U_2 & U_1 & U_1 & \varepsilon_4^0 \end{pmatrix}$$

Schrödinger equation requires that the eigenenergy ε satisfies

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

This is equivalent to

$$(\varepsilon_W - \varepsilon)^4 - 4(\varepsilon_W - \varepsilon)^2 U_1^2 + 2(\varepsilon_W - \varepsilon)^2 U_2^2 + 8(\varepsilon_W - \varepsilon)U_1^2 U_2 - 4U_1^2 U_2^2 + U_2^4 = 0$$

After factorization

$$(\varepsilon_W - \varepsilon - U_2)^2(\varepsilon_W - \varepsilon - 2U_1 + U_2)(\varepsilon_W - \varepsilon + 2U_1 + U_2) = 0$$

Therefore, the eigenenergies are

$$\begin{aligned} \varepsilon_1 &= \varepsilon_W - U_2 \\ \varepsilon_2 &= \varepsilon_W - U_2 \\ \varepsilon_3 &= \varepsilon_W + U_2 - 2U_1 \\ \varepsilon_4 &= \varepsilon_W + U_2 + 2U_1 \end{aligned}$$

2.2 Part (b)

Point U is where planes (111) and (200) meet. Therefore, there should be three corresponding k whose energies are degenerate. Let $k_1 = k_U$, $k_2 = k_U - \frac{2\pi}{a}(1,1,1)$ and $k_3 = \frac{2\pi}{a}(2,0,0)$. Their couplings are determined by

$$\begin{aligned} \vec{k}_1 - \vec{k}_2 &= \frac{2\pi}{a}(1,1,1) \to U_{111} = U_1 \\ \vec{k}_1 - \vec{k}_3 &= \frac{2\pi}{a}(2,0,0) \to U_{200} = U_2 \\ \vec{k}_2 - \vec{k}_3 &= \frac{2\pi}{a}(1,-1,-1) \to U_{1\bar{1}\bar{1}} = U_1 \end{aligned}$$

In the subspace spanned by the three plane waves, the Hamiltonian is

$$H = \begin{pmatrix} \varepsilon_1^0 & U_1 & U_2 \\ U_1 & \varepsilon_2^0 & U_1 \\ U_2 & U_1 & \varepsilon_3^0 \end{pmatrix}$$

Schrödinger equation requires that the eigenenergy ε satisfies

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

This is equivalent to

$$(\varepsilon_U - \varepsilon)^3 - 2(\varepsilon_U - \varepsilon)U_1^2 - (\varepsilon_U - \varepsilon)U_2^2 + 2U_1^2 U_2 = 0$$

After factorization

$$(\varepsilon_U - \varepsilon - U_2)\left((\varepsilon_U - \varepsilon)^2 + (\varepsilon_U - \varepsilon)U_2 - 2U_1^2\right) = 0$$

Therefore, the eigenenergies are

$$\begin{aligned}
\varepsilon_1 &= \varepsilon_U - U_2 \\
\varepsilon_2 &= \varepsilon_U + \frac{1}{2}U_2 - \frac{1}{2}\sqrt{U_2^2 + 8U_1^2} \\
\varepsilon_3 &= \varepsilon_U + \frac{1}{2}U_2 + \frac{1}{2}\sqrt{U_2^2 + 8U_1^2}
\end{aligned}$$