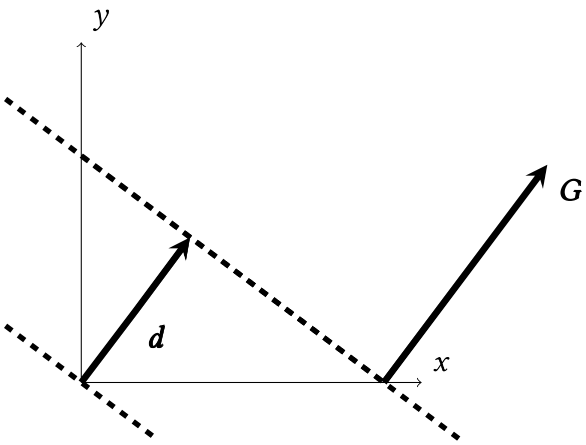

Figure 1: The interplanar separation.

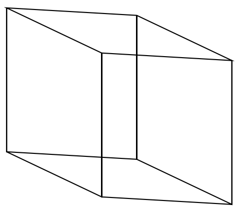

Figure 2: The first Brillouin zone of a hexagonal lattice

Quantum mechanics Assignment 1 J L Gouws
February 16, 2022 **26634554**

1.

$$(\langle\psi| + \alpha * \langle\phi|)\,(\alpha|\phi\rangle + |\psi\rangle)$$

c). The

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2. a). The volume of the primitive cell is given by:

$$V = \hat{\boldsymbol{a}}_{\boldsymbol{1}} \cdot (\hat{\boldsymbol{a}}_{\boldsymbol{2}} \times \hat{\boldsymbol{a}}_{\boldsymbol{3}})$$

We have:

$$\hat{\boldsymbol{a}}_{\boldsymbol{2}} \times \hat{\boldsymbol{a}}_{\boldsymbol{3}} = -\sqrt{3}\frac{ac}{2}(-\hat{\boldsymbol{y}}) + \frac{ac}{2}\hat{\boldsymbol{x}} = \sqrt{3}\frac{ac}{2}\hat{\boldsymbol{y}} + \frac{ac}{2}\hat{\boldsymbol{x}}$$

Thus:

$$V = \frac{\sqrt{3}a^2c}{4} + \frac{\sqrt{3}a^2c}{4} = \sqrt{3}\frac{a^2c}{2}$$

b). We have by the definition of the reciprocal lattice vectors:

$$\hat{\boldsymbol{b}_{\boldsymbol{1}}} = 2\pi\frac{\hat{\boldsymbol{a}}_{\boldsymbol{2}} \times \hat{\boldsymbol{a}}_{\boldsymbol{3}}}{V} = \frac{2\pi}{V}\begin{vmatrix} \hat{\boldsymbol{x}} & \hat{\boldsymbol{y}} & \hat{\boldsymbol{z}} \\ -\frac{\sqrt{3}a}{2} & \frac{a}{2} & 0 \\ 0 & 0 & c \end{vmatrix} = \frac{2\pi}{\sqrt{3}ac}\hat{\boldsymbol{x}} + \frac{2\pi}{a}\hat{\boldsymbol{y}}$$

$$\hat{\boldsymbol{b}_{\boldsymbol{2}}} = 2\pi\frac{\hat{\boldsymbol{a}}_{\boldsymbol{3}} \times \hat{\boldsymbol{a}}_{\boldsymbol{1}}}{V} = \frac{2\pi}{V}\begin{vmatrix} \hat{\boldsymbol{x}} & \hat{\boldsymbol{y}} & \hat{\boldsymbol{z}} \\ 0 & 0 & c \\ \frac{\sqrt{3}a}{2} & \frac{a}{2} & 0 \end{vmatrix} = -\frac{2\pi}{\sqrt{3}ac}\hat{\boldsymbol{x}} + \frac{2\pi}{a}\hat{\boldsymbol{y}}$$

$$\hat{\boldsymbol{b}_{\boldsymbol{3}}} = 2\pi\frac{\hat{\boldsymbol{a}}_{\boldsymbol{1}} \times \hat{\boldsymbol{a}}_{\boldsymbol{2}}}{V} = \frac{2\pi}{V}\begin{vmatrix} \hat{\boldsymbol{x}} & \hat{\boldsymbol{y}} & \hat{\boldsymbol{z}} \\ \frac{\sqrt{3}a}{2} & \frac{a}{2} & 0 \\ -\frac{\sqrt{3}a}{2} & \frac{a}{2} & 0 \end{vmatrix} = \frac{2\pi}{V}\frac{\sqrt{3}a^2 - (-\sqrt{3}a^2)}{2} = \frac{2\pi}{c}\hat{\boldsymbol{z}}$$

c). The first Brillouin zone is described by the planes that bisect the following vectors perpendicularly:

$$\frac{2\pi}{\sqrt{3}ac}\hat{\boldsymbol{x}} + \frac{2\pi}{a}\hat{\boldsymbol{y}}$$
$$-\frac{2\pi}{\sqrt{3}ac}\hat{\boldsymbol{x}} - \frac{2\pi}{a}\hat{\boldsymbol{y}}$$
$$-\frac{2\pi}{\sqrt{3}ac}\hat{\boldsymbol{x}} + \frac{2\pi}{a}\hat{\boldsymbol{y}}$$
$$\frac{2\pi}{\sqrt{3}ac}\hat{\boldsymbol{x}} - \frac{2\pi}{a}\hat{\boldsymbol{y}}$$
$$\pm\frac{2\pi}{c}\hat{\boldsymbol{z}}$$

This can be seen in Fig. 2, it is a rhombic prism.