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A Note on the Geometry of Lattice Planes

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This note is an attempt to give a careful restatement of a well known result in lattice geometry, the proof of the converse part of which does not appear to be so well known.

Let $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ be three non-coplanar vectors drawn from the same origin O. Any vector $\mathbf{p}$, whether drawn from O or not, is called a *lattice vector* if it can be written in the form

$$\mathbf{p} = p_1\mathbf{a}_1+p_2\mathbf{a}_2+p_3\mathbf{a}_3 , \tag{1}$$

where p_1, p_2, p_3 are any integers. Any point P whose position vector* relative to O is a lattice vector is called a *lattice point*; and the set of all such lattice points is called the *space point lattice* whose *basic vectors* or *primitive translation vectors* are $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$.

The plane through any three non-collinear lattice points P_1, P_2, P_3 is called a *lattice plane.* If P_1, P_2, P_3 are three non-collinear lattice points then their position vectors have the form

$$\mathbf{P}_i = P_{i1}\mathbf{a}_1+P_{i2}\mathbf{a}_2+P_{i3}\mathbf{a}_3, \qquad i = 1, 2, 3 , \tag{2}$$

where each P_{ij} is an integer and further det $(P_{ij}) \neq 0$ (otherwise the three points are collinear). In texts on vector algebra it is shown that the vector equation of a plane is

$$\mathbf{r}.\boldsymbol{\eta} = c , \tag{3}$$

where $\mathbf{r}$ is the position vector of any point on the plane, $\boldsymbol{\eta}$ is any vector normal to the plane and c is a constant: further $c\boldsymbol{\eta}|\boldsymbol{\eta}|^{-2}$ is the position vector of the foot of the perpendicular from O to the plane. If (3) represents the lattice plane through P_1, P_2, P_3, then

$$\mathbf{P}_1.\boldsymbol{\eta} = \mathbf{P}_2.\boldsymbol{\eta} = \mathbf{P}_3.\boldsymbol{\eta} = c , \tag{4}$$

since P_1, P_2, P_3 are points on the plane; and so

$$(\mathbf{P}_2-\mathbf{P}_3).\boldsymbol{\eta} = (\mathbf{P}_3-\mathbf{P}_1).\boldsymbol{\eta} = 0 . \tag{5}$$

Thus the point with position vector

$$\mathbf{P} = \mathbf{P}_1+\alpha_1(\mathbf{P}_2-\mathbf{P}_3)+\alpha_2(\mathbf{P}_3-\mathbf{P}_1) , \tag{6}$$

where α_1, α_2 are any real numbers, is a point on the lattice plane, as can be seen by substituting $\mathbf{P}$ in (3) and using (4) and (5). If α_1, α_2 are both integers, then $\mathbf{P}$ is a lattice vector; and since each parameter α_1, α_2 can take an enumerable infinity of integer values, each pair giving rise to a different lattice point, the plane is seen to contain a double (enumerable) infinity of lattice points not all of which lie in the same straight line. However, all the lattice points of the plane may not be given in this way by (6), as, for example, when $\frac{1}{2}(\mathbf{P}_2-\mathbf{P}_3)$ is a lattice vector. The problem of enumerating all the lattice points of a given lattice plane is not simple; it has been considered by Jaswon & Dove (1955).

If

$$\mathbf{Q}_1 = (\mathbf{P}_2-\mathbf{P}_3), \quad \mathbf{Q}_2 = (\mathbf{P}_3-\mathbf{P}_1) , \tag{7}$$

then $\mathbf{Q}_1 \wedge \mathbf{Q}_2$ is normal to the plane P_1, P_2, P_3 since, by (5),

$$(\mathbf{Q}_1 \wedge \mathbf{Q}_2) \wedge \boldsymbol{\eta} = (\mathbf{Q}_1.\boldsymbol{\eta})\mathbf{Q}_2-(\mathbf{Q}_2.\boldsymbol{\eta})\mathbf{Q}_1 = 0 .$$

Further, it can be seen that

$$\mathbf{Q}_1 \wedge \mathbf{Q}_2 = V_a(\xi_1'\mathbf{b}_1+\xi_2'\mathbf{b}_2+\xi_3'\mathbf{b}_3) , \tag{8}$$

where

$$V_a = (\mathbf{a}_1 \wedge \mathbf{a}_2).\mathbf{a}_3; \tag{9}$$

$$\mathbf{b}_i = (\mathbf{a}_j \wedge \mathbf{a}_k)/V_a, \qquad i, j, k = 1, 2, 3; \tag{10}$$

and ξ_1', ξ_2', ξ_3' are integers determined by (2). The vectors $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ are called the *reciprocal basic vectors* corresponding to the *direct basic vectors* $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$: the reciprocal basic vectors define a space point lattice called the *reciprocal lattice* corresponding to the *direct lattice* defined by $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$. Hence the lattice plane through P_1, P_2, P_3 is normal to the reciprocal-lattice vector

$$\boldsymbol{\xi}' = \xi_1\mathbf{b}_1+\xi_2'\mathbf{b}_2+\xi_3'\mathbf{b}_3 . \tag{11}$$

If $\zeta_1, \zeta_2, \zeta_3$ are relatively prime, i.e. have no common factors other than $+1$ and -1, then $\boldsymbol{\zeta} = \zeta_1\mathbf{a}_1+\zeta_2\mathbf{a}_2+\zeta_3\mathbf{a}_3$ is called a *prime* direct lattice vector (p.d.l. vector). If, further, either (i) $\zeta_1 > 0$, (ii) $\zeta_2 > 0, \zeta_1 = 0$, or (iii) $\zeta_3 > 0, \zeta_1 = \zeta_2 = 0$, then $\boldsymbol{\zeta}$ is called a *positive* prime direct lattice vector (p.p.d.l. vector). Similar definitions apply, *mutatis mutandis*, to the reciprocal lattice.

Suppose that

$$\boldsymbol{\xi} = \xi_1\mathbf{b}_1+\xi_2\mathbf{b}_2+\xi_3\mathbf{b}_3 \tag{12}$$

is the p.p.r.l. vector in the direction of $\boldsymbol{\xi}'$ of equation (11), i.e. ξ_1, ξ_2, ξ_3 are obtained from ξ_1', ξ_2', ξ_3' by

* Subsequently, all position vectors are relative to O unless another point is specified.

dividing them by their highest common factor and by (-1) if either (i) $\xi_1' < 0$, (ii) $\xi_2' < 0$ and $\xi_1' = 0$, or (iii) $\xi_3' < 0$ and $\xi_1' = \xi_2' = 0$. The equation (3) for the lattice plane P_1, P_2, P_3 may now be written

$$\mathbf{r}.\boldsymbol{\xi} = N\,, \tag{13}$$

where, since P_1 is a point on the plane and $\mathbf{a}_i.\mathbf{b}_j = \delta_{ij}$,

$$\begin{aligned} N &= \mathbf{P}_1.\boldsymbol{\xi} \\ &= P_{11}\xi_1 + P_{12}\xi_2 + P_{13}\xi_3 \\ &= \text{an integer.} \end{aligned} \tag{14}$$

If $\mathbf{r} = r_1\mathbf{a}_1 + r_2\mathbf{a}_2 + r_3\mathbf{a}_3$, then (13) may be written

$$\xi_1 r_1 + \xi_2 r_2 + \xi_3 r_3 = N\,. \tag{15}$$

It has now been shown that a lattice plane is represented by the vector equation (13), where $\boldsymbol{\xi}$ is a p.p.r.l. vector and N is an integer, both being determined by P_1, P_2, P_3. The converse result—that, for any p.p.r.l. vector $\boldsymbol{\xi}$ and any integer N, equation (13) represents a lattice plane—is not immediately obvious. It is, in fact, an elementary result in the theory of diophantine equations, but, as a proof does not appear to be current in crystallographic literature, one is now given.

Suppose that $\boldsymbol{\xi}$, as in equation (12), is a p.p.r.l. vector and that $\alpha_1', \alpha_2', \alpha_3'$ are integers such that

$$d = \alpha_1'\xi_1 + \alpha_2'\xi_2 + \alpha_3'\xi_3 \tag{16}$$

is the smallest integer greater than zero of the form

$$\alpha_1\xi_1 + \alpha_2\xi_2 + \alpha_3\xi_3\,, \tag{17}$$

where $\alpha_1, \alpha_2, \alpha_3$ are any integers. Now, by an elementary result of number theory, $\xi_1 = pd + q$, where p, q are integers and $0 \le q < d$ (see e.g. Birkhoff & MacLane, 1947). So, by equation (16),

$$q = \xi_1 - pd = (1 - p\alpha_1')\xi_1 - p\alpha_2'\xi_2 - p\alpha_3'\xi_3\,,$$

which, being in the form (17), must be zero since $0 \le q < d$ and d is the smallest integer greater than zero of the form (17). Thus $\xi_1 = pd$, and so d is a factor of ξ_1: similarly it can be shown that d is also a factor of ξ_2, ξ_3. Hence $d = 1$ since ξ_1, ξ_2, ξ_3 are relatively prime. Thus there exists three integers $\alpha_1', \alpha_2', \alpha_3'$ such that

$$\alpha_1'\xi_1 + \alpha_2'\xi_2 + \alpha_3'\xi_3 = 1\,, \tag{18}$$

and, if N is any integer,

$$(N\alpha_1')\xi_1 + (N\alpha_2')\xi_2 + (N\alpha_3')\xi_3 = N\,, \tag{19}$$

so that there exists a direct lattice point

$$\boldsymbol{\lambda} = (N\alpha_1')\mathbf{a}_1 + (N\alpha_2')\mathbf{a}_2 + (N\alpha_3')\mathbf{a}_3 \tag{20}$$

which is a point of the plane $\mathbf{r}.\boldsymbol{\xi} = N$. Further, the lattice vectors

$$\boldsymbol{\mu} = -\xi_3\mathbf{a}_2 + \xi_2\mathbf{a}_3,\quad \boldsymbol{\nu} = -\xi_2\mathbf{a}_1 + \xi_1\mathbf{a}_2 \tag{21}$$

are such that

$$\boldsymbol{\mu}.\boldsymbol{\xi} = \boldsymbol{\nu}.\boldsymbol{\xi} = 0\,, \tag{22}$$

i.e. $(0, -\xi_3, \xi_2)$ and $(-\xi_2, \xi_1, 0)$ are solutions of

$$\mathbf{r}.\boldsymbol{\xi} = r_1\xi_1 + r_2\xi_2 + r_3\xi_3 = 0\,, \tag{23}$$

as can be seen by inspection. Hence the point

$$\boldsymbol{\Lambda} = \boldsymbol{\lambda} + p\boldsymbol{\mu} + q\boldsymbol{\nu}\,, \tag{24}$$

where p, q are any numbers, lies on the plane $\mathbf{r}.\boldsymbol{\xi} = N$, since, by (19) and (22),

$$\boldsymbol{\Lambda}.\boldsymbol{\xi} = \boldsymbol{\lambda}.\boldsymbol{\xi} + p(\boldsymbol{\mu}.\boldsymbol{\xi}) + q(\boldsymbol{\nu}.\boldsymbol{\xi}) = N\,. \tag{25}$$

If p, q are both integral then $\boldsymbol{\Lambda}$ is the position vector of a lattice point lying in the plane. The plane is seen to contain a double infinity of lattice points, at least three of which are not collinear since $\boldsymbol{\mu}$ and $\boldsymbol{\nu}$ are generally not parallel: hence the plane is a lattice plane.

This completes the proof of the following theorem: *Any lattice plane of the direct lattice can be represented by the equation* $\mathbf{r}.\boldsymbol{\xi} = N$, *where* N *is some integer and* $\boldsymbol{\xi}$ *is some positive prime reciprocal lattice vector; and conversely, the equation* $\mathbf{r}.\boldsymbol{\xi} = N$, *where* N *is any integer and* $\boldsymbol{\xi}$ *is any p.p.r.l. vector, represents such a lattice plane.* The theorem is also true, *mutatis mutandis*, for the lattice planes of the reciprocal lattice.

Any plane $\mathbf{r}.\boldsymbol{\eta} = c$ is completely characterized by the vector $\boldsymbol{\eta}$ and the constant c, and may therefore be denoted by $(c; \boldsymbol{\eta})$ or $(c; \eta_1, \eta_2, \eta_3)$. The above result shows that if N is an integer and $\boldsymbol{\xi}$ is a p.p.r.l. vector, $(N; \boldsymbol{\xi})$ represents a lattice plane and that any lattice plane can be represented in this way.

The foot of the perpendicular from O to $(N; \boldsymbol{\xi})$ has position vector $N\boldsymbol{\xi}|\boldsymbol{\xi}|^{-2}$, so that the sequence of lattice planes $(N; \boldsymbol{\xi})$, $N = 0, \pm1, \pm2, \ldots$, are parallel and equally spaced a distance $|\boldsymbol{\xi}|^{-1}$ apart, with $(N; \boldsymbol{\xi})$ lying between $(N-1; \boldsymbol{\xi})$ and $(N+1; \boldsymbol{\xi})$.

If $\boldsymbol{\xi}' = n\boldsymbol{\xi}$, where n is a positive integer and $\boldsymbol{\xi}$ is a p.p.r.l. vector, then the planes of the sequence $(N; \boldsymbol{\xi}')$, $N = 0, \pm1, \pm2, \ldots$, are parallel and equally spaced a distance $|\boldsymbol{\xi}'|^{-1} = n^{-1}|\boldsymbol{\xi}|^{-1}$ apart. Those planes in this sequence for which $N = ns$, $s = 0, \pm1, \pm2, \ldots$, are the corresponding lattice planes $(s; \boldsymbol{\xi})$. Furthermore, the remaining planes of the sequence $(N; \boldsymbol{\xi}')$ cannot be lattice planes since $\mathbf{r}.\boldsymbol{\xi}' = N$ implies

$$r_1\xi_1 + r_2\xi_2 + r_3\xi_3 = N/n\,,$$

which, since in this case N/n is a fraction and ξ_1, ξ_2, ξ_3 are integers, can never be satisfied if r_1, r_2, r_3 all have integral values. The planes of the sequence $(N; \boldsymbol{\xi}')$ have the significance that they are the nodal planes of the functions $\sin \pi n(\mathbf{r}.\boldsymbol{\xi})$.

Since the lattice plane $(N; \boldsymbol{\xi})$ cuts the lines drawn from O parallel to $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ at points distant Na_1/ξ_1, Na_2/ξ_2, Na_3/ξ_3 from O, the *Miller indices* relative to $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ of the plane are proportional to ξ_1, ξ_2, ξ_3 and hence, by the theorem proved here, are proportional to integers.

References

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