GENERALIZED CRYSTALS **IN PROGRESS**

Thomas Wieting
Reed College, 2010

1 Introduction

01° One can describe *classical crystals* either in terms of tempered measures on the real space $\mathbf{R}^3$ comprised of position vectors or in terms of tempered measures on the reciprocal space $\mathbf{R}^3$ comprised of wave vectors. The two descriptions are related by the Fourier Transform. We explain these matters in the following five sections. With reference to the work of N. D. Mermin and his collaborators, we then propose a definition of *generalized crystal*. This definition takes form not in real space but in reciprocal space. Finally, we seek significant relations between the proposed generalized crystals in reciprocal space and the familiar Delone sets and quasicrystals in real space.

2 Lattices

02° Let us introduce the standard basis vectors for $\mathbf{R}^3$:

$$E_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad E_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad E_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

By a *lattice* $\mathbf{L}$ in the real space $\mathbf{R}^3$, one means a subset of $\mathbf{R}^3$ of the form:

$$\mathbf{L} := \mathcal{L}(\mathbf{Z}^3)$$

where $\mathcal{L}$ is any invertible linear mapping carrying $\mathbf{R}^3$ to itself. The vectors:

$$F_j = \mathcal{L}(E_j) \qquad (1 \leq j \leq 3)$$

form a lattice basis for $\mathbf{L}$.

03° By the lattice $\mathbf{M}$ in the reciprocal space $\mathbf{R}^3$ *reciprocal* to $\mathbf{L}$, one means the corresponding subset of $\mathbf{R}^3$:

$$\mathbf{M} := (\mathcal{L}^{-1})^*(\mathbf{Z}^3)$$

This lattice figures in the X-ray analysis of classical crystals. The vectors:

$$G_j = (\mathcal{L}^{-1})^*(E_j) \qquad (1 \leq j \leq 3)$$

form a lattice basis for $\mathbf{M}$.

04° Let us take a moment to be careful. We have presented $\mathbf{L}$ and $\mathbf{M}$ in terms of $\mathcal{L}$. We need to show that, for any invertible linear mappings $\mathcal{L}_1$ and $\mathcal{L}_2$ carrying $\mathbf{R}^3$ to itself, if $\mathcal{L}_1(\mathbf{Z}^3) = \mathcal{L}_2(\mathbf{Z}^3)$, so that $\mathcal{L}_1$ and $\mathcal{L}_2$ define the same lattice $\mathbf{L}$ in the real space $\mathbf{R}^3$, then $(\mathcal{L}_1^{-1})^*(\mathbf{Z}^3) = (\mathcal{L}_2^{-1})^*(\mathbf{Z}^3)$, so that $(\mathcal{L}_1^{-1})^*$ and $(\mathcal{L}_2^{-1})^*$ define the same lattice $\mathbf{M}$ in the reciprocal space $\mathbf{R}^3$. To that end, let $\mathcal{Z}$ be the invertible linear mapping $\mathcal{L}_2^{-1}\mathcal{L}_1$ carrying $\mathbf{R}^3$ to itself. Clearly, $\mathcal{Z}(\mathbf{Z}^3) = \mathbf{Z}^3$. One can easily check that, $(\mathcal{Z}^{-1})^* = ((\mathcal{L}_2^{-1})^*)^{-1}(\mathcal{L}_1^{-1})^*$. Of course, $(\mathcal{Z}^{-1})^*(\mathbf{Z}^3) = \mathbf{Z}^3$. Hence, $(\mathcal{L}_1^{-1})^*(\mathbf{Z}^3) = (\mathcal{L}_2^{-1})^*(\mathbf{Z}^3)$.

05° For any U and V in $\mathbf{R}^3$:

$$U \bullet V = \mathcal{L}(U) \bullet (\mathcal{L}^{-1})^*(V) = X \bullet Y$$

where $X = \mathcal{L}(U)$ and $Y = (\mathcal{L}^{-1})^*(V)$. By this fact, one can see all the more clearly the special relation between $\mathbf{L}$ and $\mathbf{M}$. Thus, for any Y in $\mathbf{R}^3$, $Y \in \mathbf{M}$ iff, for any X in $\mathbf{L}$, $X \bullet Y \in \mathbf{Z}$. Moreover:

$$F_j \bullet G_k = \delta_{jk} \qquad (1 \leq j \leq 3,\ 1 \leq k \leq 3)$$

06° Let Y be any vector in $\mathbf{M}$ for which $Y \neq 0$. Let y^1, y^2, and y^3 be the (integral) coordinates for Y relative to the prescribed lattice basis for $\mathbf{M}$:

$$Y = y^k G_k$$

Let us assume that the gcd of these integers is 1. For each ℓ in $\mathbf{Z}$, let $\mathbf{H}_\ell(Y)$ be the lattice *hyperplane* in $\mathbf{L}$ comprised of all vectors X in $\mathbf{L}$ for which:

$$X \bullet Y = \ell$$

These hyperplanes, all nonempty, lie parallel to one another. The spacing is measured by the reciprocal of the length of Y:

$$\frac{1}{\sqrt{Y \bullet Y}}$$

The collective:

$$\mathbf{H}_\ell(Y) \qquad (\ell \in \mathbf{Z})$$

of lattice hyperplanes exhausts $\mathbf{L}$:

$$\mathbf{L} = \bigcup_{\ell \in \mathbf{Z}} \mathbf{H}_\ell(Y)$$

The ordered triple (y^1, y^2, y^3) is called the *Miller Index* for the collective. See the following Figure, which displays an example of $\mathbf{L}$ and $\mathbf{M}$, reduced in dimension to $\mathbf{R}^2$.

Figure 1

3 Crystallographic Groups

07° For smooth expression, we require certain terminology and notation. First, let $\mathbf{G}$ stand for the group of all invertible linear mappings carrying $\mathbf{R}^3$ to itself. For each T in $\mathbf{R}^3$ and for each Λ in $\mathbf{G}$, we introduce the *affine* mapping:

$$[T, \Lambda]$$

carrying $\mathbf{R}^3$ to itself. For each X in $\mathbf{R}^3$:

$$[T, \Lambda](X) = T + \Lambda(X)$$

We refer to T as the *translational* part and to Λ as the *linear* part of $[T, \Lambda]$. Clearly, $[T, \Lambda]$ is invertible. The family $\mathbf{A}$ of all such mappings forms a group under composition, since the following relations prevail:

$$[T_1, \Lambda_1][T_2, \Lambda_2] = [T_1 + \Lambda_1(T_2), \Lambda_1\Lambda_2]$$
$$[T, \Lambda]^{-1} = [-\Lambda^{-1}(T), \Lambda^{-1}]$$

Of course, the identity in $\mathbf{A}$ is $I = [0, I]$, where I is the identity in $\mathbf{G}$.

08° Let us label several basic subgroups of $\mathbf{A}$. Let $\mathbf{O}$ be the subgroup of $\mathbf{G}$ comprised of all invertible linear mappings Λ which are orthogonal and let $\mathbf{C}$ be the subgroup of $\mathbf{A}$ comprised of all affine mappings $[T, \Lambda]$ for which $\Lambda \in \mathbf{O}$. One refers to the latter as *Cartesian* mappings. Let $\mathbf{H}$ be the subgroup of $\mathbf{G}$

comprised of all invertible linear mappings Λ under which the standard lattice $\mathbf{Z}^3$ is invariant:

$$\Lambda(\mathbf{Z}^3) = \mathbf{Z}^3$$

Let $\mathbf{G}^+$ be the subgroup of $\mathbf{G}$ comprised of all Λ for which $0 < det(\Lambda)$ and let $\mathbf{A}^+$ be the subgroup of $\mathbf{A}$ comprised of all $[T, \Lambda]$ for which $\Lambda \in \mathbf{G}^+$. Let $\mathbf{O}^+ = \mathbf{O} \cap \mathbf{G}^+$, let $\mathbf{C}^+ = \mathbf{C} \cap \mathbf{A}^+$, and, finally, let $\mathbf{H}^+ = \mathbf{H} \cap \mathbf{G}^+$.

09° For any subgroup $\mathbf{B}$ of $\mathbf{A}$, we introduce the *translational* part $\mathbf{T}$ of $\mathbf{B}$, comprised of all T in $\mathbf{R}^3$ for which $[T, I] \in \mathbf{B}$; and we introduce the *linear* part $\mathbf{\Lambda}$ of $\mathbf{B}$, comprised of all Λ in $\mathbf{G}$ for which there is some $\bar{T}$ in $\mathbf{R}^3$ such that $[\bar{T}, \Lambda] \in \mathbf{B}$. Clearly, $\mathbf{T}$ is a subgroup of $\mathbf{R}^3$ and $\mathbf{\Lambda}$ is a subgroup of $\mathbf{G}$. We claim that $\mathbf{T}$ is invariant under $\mathbf{\Lambda}$. To prove the claim, we note that, for each Λ in $\mathbf{\Lambda}$, there is some $\bar{T}$ in $\mathbf{R}^3$ such that $[\bar{T}, \Lambda]$ lies in $\mathbf{B}$. Hence:

$$[\bar{T}, \Lambda][T, I][\bar{T}, \Lambda]^{-1} = [\Lambda(T), I]$$

We infer that $\Lambda(T)$ lies in $\mathbf{T}$. We conclude that $\mathbf{T}$ is *invariant* under $\mathbf{\Lambda}$.

10° Let $\mathbf{B}$ be a subgroup of $\mathbf{A}$. Let $\mathbf{T}$ be the translational part and let $\mathbf{\Lambda}$ be the linear part of $\mathbf{B}$. We can present these groups neatly in a short exact sequence:

$$\mathbf{T} \xrightarrow{\theta} \mathbf{B} \xrightarrow{\phi} \mathbf{\Lambda}$$

where, for each T in $\mathbf{T}$:

$$\theta(T) = [T, I]$$

and where, for each $[\bar{T}, \Lambda]$ in $\mathbf{B}$:

$$\phi([\bar{T}, \Lambda]) = \Lambda$$

11° Let $\mathbf{\Omega}$ be the quotient group $\mathbf{R}^3/\mathbf{T}$. Let ρ be the natural homomorphism carrying $\mathbf{R}^3$ to $\mathbf{\Omega}$:

$$\rho(V) = V + \mathbf{T}$$

where V is any position vector in $\mathbf{R}^3$. For any Λ in $\mathbf{\Lambda}$, we can define the (quotient) isomorphism $\hat{\Lambda}$ carrying $\mathbf{\Omega}$ to itself, as follows:

$$\hat{\Lambda}(V + \mathbf{T}) = \Lambda(V) + \mathbf{T}$$

where V is any position vector in $\mathbf{R}^3$. Obviously:

$$\hat{\Lambda}\rho = \rho\Lambda$$

12° For each Λ in $\mathbf{\Lambda}$, let $\gamma(\Lambda)$ be the subset $\mathbf{R}^3$ comprised of all position vectors $\bar{T}$ such that $[\bar{T}, \Lambda] \in \mathbf{B}$. Clearly, $\gamma(\Lambda)$ is a coset of $\mathbf{T}$ in $\mathbf{R}^3$. Hence, we can interpret γ as a mapping carrying $\mathbf{\Lambda}$ to $\mathbf{\Omega}$. One can easily check that γ meets the condition:

$$\gamma(\Lambda'\Lambda'') = \gamma(\Lambda') + \hat{\Lambda}'(\gamma(\Lambda''))$$

where Λ' and Λ'' are any members of $\mathbf{\Lambda}$. One refers to such a mapping as a 1-*cocycle*.

13° In brief, the subgroup $\mathbf{B}$ of $\mathbf{A}$ defines the ordered triple:

$$\mathbf{B} \longrightarrow (\mathbf{T}, \mathbf{\Lambda}, \gamma)$$

where $\mathbf{T}$ is the translational part and $\mathbf{\Lambda}$ is the linear part of $\mathbf{B}$, and where γ is the corresponding 1-cocycle carrying $\mathbf{\Lambda}$ to $\mathbf{\Omega} = \mathbf{R}^3/\mathbf{T}$. By definition, one can recover $\mathbf{B}$ from $(\mathbf{T}, \mathbf{\Lambda}, \gamma)$. In fact, for each $[\bar{T}, \Lambda]$ in $\mathbf{A}$:

$$(*) \qquad [\bar{T}, \Lambda] \in \mathbf{B} \quad \text{iff} \quad \Lambda \in \mathbf{\Lambda} \ \text{ and } \ \bar{T} \in \gamma(\Lambda)$$

14° Conversely, let $(\mathbf{T}, \mathbf{\Lambda}, \gamma)$ be an ordered triple for which $\mathbf{T}$ is a subgroup of $\mathbf{R}^3$, $\mathbf{\Lambda}$ is a subgroup of $\mathbf{G}$ under which $\mathbf{T}$ is invariant, and γ is a 1-cocycle carrying $\mathbf{\Lambda}$ to $\mathbf{\Omega} = \mathbf{R}^3/\mathbf{T}$. By invoking the foregoing condition $(*)$, one can define a subgroup $\mathbf{B}$ of $\mathbf{A}$, which in turn defines $(\mathbf{T}, \mathbf{\Lambda}, \gamma)$.

15° Obviously, the correspondence between subgroups $\mathbf{B}$ of $\mathbf{A}$ and ordered triples $(\mathbf{T}, \mathbf{\Lambda}, \gamma)$ is bijective.

16° Let us note the significant case in which $\mathbf{B}$ is the *semi-direct product* of $\mathbf{T}$ and $\mathbf{\Lambda}$:

$$\mathbf{B} = \mathbf{T} \leftthreetimes \mathbf{\Lambda}$$

The members of $\mathbf{B}$ are the affine mappings $[T, \Lambda]$ such that $T \in \mathbf{T}$ and $\Lambda \in \mathbf{\Lambda}$. The corresponding 1-cocycle γ is constant:

$$\gamma(\Lambda) = \mathbf{T}$$

where Λ is any member of $\mathbf{\Lambda}$.

17° For later reference, let us describe the relation of conjugacy for subgroups of $\mathbf{A}$ in terms of the corresponding ordered triples. Thus, let $\mathbf{B}_1$ and $\mathbf{B}_2$ be subgroups of $\mathbf{A}$ and let $(\mathbf{T}_1, \mathbf{\Lambda}_1, \gamma_1)$ and $(\mathbf{T}_2, \mathbf{\Lambda}_2, \gamma_2)$ be the corresponding ordered triples. For any $[T, L]$ in $\mathbf{A}$, we have:

$$\mathbf{B}_2 = [T, L]\mathbf{B}_1[T, L]^{-1}$$

iff:

$$\mathbf{T}_2 = L(\mathbf{T}_1)$$
$$\mathbf{\Lambda}_2 = L\mathbf{\Lambda}_1 L^{-1}$$
$$\gamma_2 = [T, L] \cdot \gamma_1$$

The last of the foregoing relations means that, for any Λ_2 in $\mathbf{\Lambda}_2$:

$$([T, L] \cdot \gamma_1)(\Lambda_2) = (\Omega_2 - \hat{\Lambda}_2(\Omega_2)) + \hat{L}(\gamma_1(L^{-1}\Lambda_2 L)$$

where $\Omega_2 = \rho_2(T) = T + \mathbf{T}_2$.

18° These relations suggest the following action of $\mathbf{A}$ on ordered triples. For any $[T, L]$ in $\mathbf{A}$ and for any ordered triple $(\mathbf{T}, \mathbf{\Lambda}, \gamma)$:

$$[T, L] \cdot (\mathbf{T}, \mathbf{\Lambda}, \gamma) = (L(\mathbf{T}), L\mathbf{\Lambda}L^{-1}, [T, L] \cdot \gamma)$$

For each Λ in $L\mathbf{\Lambda}L^{-1}$:

$$([T, L] \cdot \gamma)(\Lambda) = (\Omega - \hat{\Lambda}(\Omega)) + \hat{L}(\gamma(L^{-1}\Lambda L)$$

where $\Omega = T + L(\mathbf{T})$ and where $\hat{\Lambda}(\Omega) = \Lambda(T) + L(\mathbf{T})$.

19° Clearly, the subgroups $\mathbf{B}_1$ and $\mathbf{B}_2$ of $\mathbf{A}$ are conjugate in $\mathbf{A}$ iff the corresponding ordered triples $(\mathbf{T}_1, \mathbf{\Lambda}_1, \gamma_1)$ and $(\mathbf{T}_2, \mathbf{\Lambda}_2, \gamma_2)$ lie in the same orbit under the action of $\mathbf{A}$.

20° By a *crystallographic group*, one means any subgroup $\mathbf{B}$ of $\mathbf{C}$ such that the translational part $\mathbf{T}$ of $\mathbf{B}$ is a lattice in $\mathbf{R}^3$. Of course, the linear part $\mathbf{\Lambda}$ of $\mathbf{B}$ is a subgroup of $\mathbf{O}$. One refers to $\mathbf{T}$ as the *lattice* and to $\mathbf{\Lambda}$ as the *point group* for $\mathbf{B}$.

21° Since $\mathbf{T}$ is invariant under $\mathbf{\Lambda}$, $\mathbf{\Lambda}$ must be finite. Moreover, for each Λ in $\mathbf{\Lambda}$, $tr(\Lambda) \in \mathbf{Z}$. It follows that, for each (rotation) Λ in $\mathbf{\Lambda} \cap \mathbf{O}^+$, the order of Λ must equal 1, 2, 3, 4, or 6. This condition is the celebrated *Crystallographic Restriction*.

22° The first objective of Mathematical Crystallography is to classify the crystallographic groups under various natural equivalence relations. The least restrictive instance of such relations is the relation of isomorphism. Thus, for any crystallographic groups $\mathbf{B}'$ and $\mathbf{B}''$, one says that $\mathbf{B}'$ and $\mathbf{B}''$ are *equivalent* iff they are isomorphic. By the Theorem of Bieberbach, $\mathbf{B}'$ and $\mathbf{B}''$ are isomorphic iff they are conjugate in $\mathbf{A}$. By systematic computation, one finds that there are 219 isomorphism classes, organized by a hierarchy of 14 forms of lattices in $\mathbf{R}^3$ and a typology of 32 conjugacy classes of finite

subgroups of **O**. One calls the former the **Bravais Lattices** and the latter the **Point Groups**.

23° Let us sketch the computations required to find the isomorphism classes of crystallographic groups. To that end, let us introduce a more flexible definition of crystallographic group. Let **B** be any subgroup of **A**. Let us say that **B** is a *crystallographic* group* iff the translational part **T** of **B** is a lattice in $\mathbf{R}^3$ and the linear part $\mathbf{\Lambda}$ of **B** is finite. For such a group **B**, one can easily show that there are crystallographic* subgroups $\mathbf{B}_1$ and $\mathbf{B}_2$ of **A** such that $\mathbf{B}_1$, **B**, and $\mathbf{B}_2$ are mutually conjugate in **A** and such that $\mathbf{\Lambda}_1 \subseteq \mathbf{O}$ and $\mathbf{T}_2 = \mathbf{Z}^3$. Of course, $\mathbf{\Lambda}_2 \subseteq \mathbf{H}$. Clearly, $\mathbf{B}_1$ is a crystallographic group in the conventional sense. Hence, for the objective of classification by isomorphism, the more flexible definition yields no unwarranted equivalence classes. However, the definition directs attention to the groups $\mathbf{B}_2$ for which $\mathbf{T}_2 = \mathbf{Z}^3$ and $\mathbf{\Lambda}_2 \subseteq \mathbf{H}$. For such groups, we can compute the isomorphism classes in terms, essentially, of integer arithmetic.

24° ..... Details in Burckhardt.

25° For the crystallographer, the crystallographic groups $\mathbf{B}'$ and $\mathbf{B}''$ are equivalent iff they are conjugate in $\mathbf{A}^+$. Under this slightly more refined relation, designed to respect orientation, each of eleven of the foregoing isomorphism classes breaks into two subclasses. Hence, for the crystallographer, there are 230 equivalence classes of crystallographic groups.

4 Tempered Measures

26° Let $\mathcal{A}$ stand for the family of all Borel subsets of $\mathbf{R}^3$ and let $\mathcal{B}$ stand for the subfamily of $\mathcal{A}$ comprised of all bounded Borel subsets of $\mathbf{R}^3$. For our development of classical and of generalized crystals, we require complex valued measures μ defined on $\mathcal{B}$. For such a measure μ, let us emphasize the requirement that, for any sequence:

$$B_1,\ B_2,\ B_3,\ \ldots$$

of mutually disjoint sets in $\mathcal{B}$, if:

$$\bigcup_{j=1}^{\infty} B_j$$

lies in $\mathcal{B}$ then:

$$\mu(\bigcup_{j=1}^{\infty} B_j) = \sum_{j=1}^{\infty} \mu(B_j)$$

27° For any nonnegative real valued measure ν defined on $\mathcal{B}$, one can, by routine argument, introduce a nonnegative extended real valued measure $\nu^\bullet$

defined on $\mathcal{A}$ such that, for any B in $\mathcal{B}$, $\nu^\bullet(B) = \nu(B)$. In practice, one simply identifies ν and $\nu^\bullet$:

$$\nu = \nu^\bullet$$

28° Given a complex valued measure μ defined on $\mathcal{B}$, one can introduce the nonnegative real valued measure $|\mu|$ defined on $\mathcal{B}$, called the *total variation* of μ. It is characterized by the condition that, for any nonnegative real valued measure ν defined on $\mathcal{B}$, if, for any B in $\mathcal{B}$:

$$|\mu(B)| \leq \nu(B)$$

then, for any B in $\mathcal{B}$:

$$|\mu|(B) \leq \nu(B)$$

29° Now let f be any complex valued Borel function defined on $\mathbf{R}^3$. One says that f is *tempered* iff, for each positive integer ℓ, there is a positive real number C such that, for each X in $\mathbf{R}^3$:

$$(1 + X \bullet X)^\ell \, |f(X)| \, \leq \, C$$

Let $\mathcal{F}$ stand for the family of all such functions.

30° Let μ be a complex valued measure defined on $\mathcal{B}$. One says that μ is *tempered* iff there is some positive integer ℓ such that:

$$\int_{\mathbf{R}^3} (1 + X \bullet X)^{-\ell} \, |\mu|(dX) \, < \, \infty$$

For such a measure and for each f in $\mathcal{F}$:

$$\int_{\mathbf{R}^3} |f|(X) \, |\mu|(dX) \, < \, \infty$$

Moreover, the following integral would have precise meaning:

$$\int_{\mathbf{R}^3} f(X) \, \mu(dX)$$

Consequently, one may interpret the tempered measure μ as a linear functional on the linear space $\mathcal{F}$ of all tempered functions.

31° Clearly, the Lebesgue measure λ defined on $\mathcal{B}$ is tempered.

32° Let μ be a complex valued measure defined on $\mathcal{B}$. One says that μ has *bounded support* iff there is some A in $\mathcal{B}$ such that:

$$|\mu|(\mathbf{R}^3 \backslash A) = 0$$

That is, for any B in $\mathcal{B}$, if $A \cap B = \emptyset$ then $\mu(B) = 0$. Let us write:

$$supp(\mu) \subseteq A$$

to express this condition. Obviously, if μ has bounded support then μ is tempered.

33° Now let $\mathbf{K}$ be a closed discrete, hence countable subset of $\mathbf{R}^3$. Let $\delta_{\mathbf{K}}$ be the nonnegative real valued measure defined on $\mathcal{B}$ such that, for each X in $\mathbf{K}$:

$$\delta_{\mathbf{K}}(\{X\}) = 1$$

while, for any B in $\mathcal{B}$, if $\mathbf{K} \cap B = \emptyset$ then $\delta_{\mathbf{K}}(B) = 0$. One refers to $\delta_{\mathbf{K}}$ as the *dirac comb* defined by $\mathbf{K}$.

34° One says that $\mathbf{K}$ is a *Delone* subset of $\mathbf{R}^3$ iff there exist positive real numbers r and R such that, for any open ball B in $\mathbf{R}^3$, if the radius of B is less than r then B contains at most one member of $\mathbf{K}$, while if the radius of B is greater than R then B contains at least one member of $\mathbf{K}$. For example, $\mathbf{K}$ might be the union of a finite family of cosets of a lattice $\mathbf{L}$ in $\mathbf{R}^3$:

$$\mathbf{K} = \bigcup_{j=1}^{k} (S_j + \mathbf{L})$$

where:

$$S_1, S_2, \ \ldots \ , S_k$$

are any position vectors in $\mathbf{R}^3$. In any case, if $\mathbf{K}$ is a Delone set then:

$$\int_{\mathbf{R}^3} (1 + X \bullet X)^{-3} \, \delta_{\mathbf{K}}(dX) = \sum_{X \in \mathbf{K}} (1 + X \bullet X)^{-3} \ < \ \infty$$

Hence, $\delta_{\mathbf{K}}$ is tempered and, for each tempered function f defined on $\mathbf{R}^3$:

$$\int_{\mathbf{R}^3} f(X) \delta_{\mathbf{K}}(dX) = \sum_{X \in \mathbf{K}} f(X)$$

35° For any tempered function f defined on $\mathbf{R}^3$ and for any affine mapping $[T, \Lambda]$ carrying $\mathbf{R}^3$ to itself, we define the *transform*:

$$[T, \Lambda] \cdot f$$

of f by $[T, \Lambda]$ as follows:

$$([T, \Lambda] \cdot f)(X) = f([T, \Lambda]^{-1}(X))$$

where X is any position vector in $\mathbf{R}^3$. Clearly, $[T, \Lambda] \cdot f$ is a tempered function defined on $\mathbf{R}^3$. As usual, we find the following relations for a group operating upon a set:

$$([T_1, \Lambda_1][T_2, \Lambda_2]) \cdot f = [T_1, \Lambda_1] \cdot ([T_2, \Lambda_2] \cdot f)$$
$$[0, I] \cdot f = f$$

36° In turn, for any complex valued measure μ defined on $\mathcal{B}$ and for any affine mapping $[T, \Lambda]$ carrying $\mathbf{R}^3$ to itself, we define the *transform*:

$$[T, \Lambda] \cdot \mu$$

of μ by $[T, \Lambda]$ as follows:

$$[T, \Lambda] \cdot \mu = [T, \Lambda]_*(\mu)$$

That is, for any B in $\mathcal{B}$:

$$([T, \Lambda] \cdot \mu)(B) = \mu([T, \Lambda]^{-1}(B))$$

Clearly, $[T, \Lambda] \cdot \mu$ is a complex valued measure defined on $\mathcal{B}$. Again, we find the following relations for a group operating upon a set:

$$([T_1, \Lambda_1][T_2, \Lambda_2]) \cdot \mu = [T_1, \Lambda_1] \cdot ([T_2, \Lambda_2] \cdot \mu)$$
$$[0, I] \cdot \mu = \mu$$

37° For later reference, we note that, for any tempered function f, for any tempered measure μ, and for any affine mapping $[T, L]$:

$$\int_{\mathbf{R}^3} ([T, L]^{-1} \cdot f)(X)\mu(dX) = \int_{\mathbf{R}^3} f(X)([T, L] \cdot \mu)(dX)$$

38° Finally, let μ be a complex valued measure defined on $\mathcal{B}$. Let us denote by $\mathbf{C}_\mu$ the stabilizer of μ in $\mathbf{C}$. That is, for any $[T, \Lambda]$ in $\mathbf{C}$:

$$[T, \Lambda] \in \mathbf{C}_\mu \quad \text{iff} \quad [T, \Lambda] \cdot \mu = \mu$$

Of course, $\mathbf{C}_\mu$ is a subgroup of $\mathbf{C}$. One refers to $\mathbf{C}_\mu$ as the *symmetry* group of μ. Let us denote the translational part of $\mathbf{C}_\mu$ by $\mathbf{T}_\mu$ and the linear part of $\mathbf{C}_\mu$ by $\mathbf{\Lambda}_\mu$. Again, we can present these significant groups neatly in a short exact sequence:

$$\mathbf{T}_\mu \xrightarrow{\theta} \mathbf{C}_\mu \xrightarrow{\phi} \mathbf{\Lambda}_\mu$$

5 Classical Crystals

39° Now we are prepared to describe the basic concept of our subject. By a *classical crystal*, we mean a nonnegative real valued measure ν defined on $\mathcal{B}$ such that the symmetry group $\mathbf{C}_\nu$ of ν is a crystallographic group. One refers to $\mathbf{T}_\nu$ as the *lattice* and to $\mathbf{\Lambda}_\nu$ as the *point group* for the classical crystal ν.

40° For the methods of X-ray crystallography, the identification of a classical crystal with a nonnegative measure seems to be adequate. For any B in $\mathcal{B}$, one interprets $\nu(B)$ to be the number of electrons contained in B. Hence, the measure serves as a model for the distribution of electrons within the crystal. It seems that the electrons play the dominant role in the scattering of X-ray radiation and hence in the forming of diffraction patterns. Of course, for other experimental methods, one invokes other models.

41° For any classical crystals ν' and ν'', one says that ν' and ν'' are *equivalent* iff the symmetry groups $\mathbf{C}_{\nu'}$ and $\mathbf{C}_{\nu''}$ are conjugate in $\mathbf{A}^+$. We hasten to note that, for any crystallographic group $\mathbf{B}$, there is some classical crystal ν such that:

$$\mathbf{C}_\nu = \mathbf{B}$$

Indeed, one can take ν to be a Dirac comb:

$$\nu = \delta_{\mathbf{K}}$$

where $\mathbf{K}$ is the union of a suitable finite family of cosets of a lattice $\mathbf{L}$ in $\mathbf{R}^3$. In any case, there are 230 equivalence classes of classical crystals. Nature has grown instances of some of such classes but not of others. Later, we will describe the instance of the diamond crystal, an especially interesting case.

42° For any classical crystals ν' and ν'', one says that ν' and ν'' are *congruent* iff there is a Cartesian mapping $[T, \Lambda]$ in $\mathbf{C}^+$ such that $\nu'' = [T, \Lambda] \cdot \nu'$. One may say that such classical crystals ν' and ν'' are physically indistinguishable. Of course:

$$\mathbf{C}_{\nu''} = [T, \Lambda]\mathbf{C}_{\nu'}[T, \Lambda]^{-1}$$

so that ν' and ν'' are equivalent.

43° Let ν be any classical crystal and let $\mathbf{L} = \mathbf{T}_\nu$ be the lattice of translational symmetries of ν. Let $\mathbf{J}$ be a *cross section* for $\mathbf{L}$. By definition, $\mathbf{J} \in \mathcal{B}$ and the sets:

$$[X, I](\mathbf{J}) \qquad (X \in \mathbf{L})$$

form a partition of $\mathbf{R}^3$. Very often, but not always we take $\mathbf{J}$ to be a *basic parallelopiped* for $\mathbf{L}$:

$$\mathbf{J} = \mathcal{L}(\mathbf{I})$$

where $\mathcal{L}$ is an invertible linear mapping carrying $\mathbf{R}^3$ to itself for which:

$$\mathbf{L} = \mathcal{L}(\mathbf{Z}^3)$$

and where $\mathbf{I}$ is the standard unit cube in $\mathbf{R}^3$, comprised of the position vectors:

$$U = U^j E_j$$

for which:

$$0 \leq U^j < 1 \qquad (1 \leq j \leq 3)$$

44° Let n be the restriction of ν to $\mathbf{J}$:

$$n(B) = \nu(\mathbf{J} \cap B)$$

where B is any set in $\mathcal{B}$. Obviously, $supp(n) \subseteq \mathbf{J}$. We refer to n as the *local electron distribution* for the classical crystal ν, relative to $\mathbf{J}$. To distinguish n and ν, we refer to ν itself as the *global electron distribution*.

45° For each B in $\mathcal{B}$:

$$\begin{aligned}
\nu(B) &= \nu(\bigcup_{X \in \mathbf{L}} [X, I](\mathbf{J}) \cap B) \\
&= \sum_{X \in \mathbf{L}} \nu([X, I](\mathbf{J}) \cap B) \\
&= \sum_{X \in \mathbf{L}} \nu(\mathbf{J} \cap [X, I]^{-1}(B)) \quad \text{(because } [X, I] \cdot \nu = \nu) \\
&= \sum_{X \in \mathbf{L}} n([X, I]^{-1}(B)) \\
&= \sum_{X \in \mathbf{L}} \int_{\mathbf{J}} ch_{[X,I]^{-1}(B)}(W) n(dW) \\
&= \int_{\mathbf{R}^3} \int_{\mathbf{J}} ch_B(W + X) n(dW) \delta_{\mathbf{L}}(dX)
\end{aligned}$$

Hence, the global electron distribution ν for a classical crystal is the convolution of the local electron distribution n (relative to a selected cross section $\mathbf{J}$ for $\mathbf{L}$) and the Dirac comb $\delta_{\mathbf{L}}$ defined by $\mathbf{L}$:

$$\begin{aligned}
\nu &= n * \delta_{\mathbf{L}} \\
&= \sum_{X \in \mathbf{L}} [X, I] \cdot n
\end{aligned}$$

46° For any W and X in $\mathbf{R}^3$:

$$2\,W \bullet X \;\leq\; 2\,W \bullet X + (W-X) \bullet (W-X) \;=\; W \bullet W + X \bullet X$$

Hence:

$$(1 + (W+X) \bullet (W+X)) \;\leq\; 2(1 + W \bullet W)(1 + X \bullet X)$$

Replacing first X by $X - W$ and then W by $-W$, we find that:

$$(1 + X \bullet X) \;\leq\; 2(1 + W \bullet W)(1 + (W+X) \bullet (W+X))$$

That is:

$$(1 + (W+X) \bullet (W+X))^{-1} \;\leq\; 2(1 + W \bullet W)(1 + X \bullet X)^{-1}$$

Hence:

$$\begin{aligned}
&\int_{\mathbf{R}^3} (1 + V \bullet V)^{-3}\, \nu(dV) \\
&\qquad = \int_{\mathbf{R}^3} \int_{\mathbf{J}} (1 + (W+X) \bullet (W+X))^{-3} n(dW) \delta_{\mathbf{L}}(dX) \\
&\qquad = \int_{\mathbf{R}^3} \int_{\mathbf{J}} 8(1 + W \bullet W)^3 (1 + X \bullet X)^{-3} n(dW) \delta_{\mathbf{L}}(dX) \\
&\qquad < \infty
\end{aligned}$$

It follows that ν is tempered. Moreover, for any tempered function f defined on $\mathbf{R}^3$:

$$\begin{aligned}
\int_{\mathbf{R}^3} f(V) \nu(dV) &= \int_{\mathbf{R}^3} \int_{\mathbf{J}} f(W+X) n(dW) \delta_{\mathbf{L}}(dX) \\
&= \sum_{X \in \mathbf{L}} \int_{\mathbf{J}} f(W+X) n(dW)
\end{aligned}$$

47° For later reference, we note that, for any affine mapping $[T, \Lambda]$ carrying $\mathbf{R}^3$ to itself:

$$[T, \Lambda] \cdot \nu = ([T, \Lambda] \cdot n) * ([0, \Lambda] \cdot \delta_{\mathbf{L}}) = ([T, \Lambda] \cdot n) * \delta_{\Lambda(\mathbf{L})}$$

In particular:

$$[T, I] \cdot \nu = ([T, I] \cdot n) * \delta_{\mathbf{L}}$$

48° Let us introduce the compact Abelian quotient group $\mathbf{\Omega}$:

$$\mathbf{\Omega} = \mathbf{R}^3 / \mathbf{L}$$

together with the natural homomorphism ρ carrying $\mathbf{R}^3$ to $\mathbf{\Omega}$:

$$\rho(V) = V + \mathbf{L}$$

where V is any position vector in $\mathbf{R}^3$. We replace n by its image σ under ρ:

$$\sigma = \rho_*(n)$$

Now we may regard σ as the local electron distribution. In fact, since the restriction of ρ to $\mathbf{J}$ is bijective, σ contains the same information as n. Let us show that σ remains unchanged though $\mathbf{J}$ be varied. To that end, let $\mathbf{J}_1$ and $\mathbf{J}_2$ be any cross sections for $\mathbf{L}$ and let n_1 and n_2 be the corresponding local electron distributions. For each B in $\mathcal{B}$:

$$\begin{aligned}
\rho_*(n_1)(B + \mathbf{L}) &= n_1(B + \mathbf{L}) \\
&= \nu(\mathbf{J}_1 \cap (B + \mathbf{L})) \\
&= \nu(\bigcup_{X \in \mathbf{L}} [X, I](\mathbf{J}_2) \cap \mathbf{J}_1 \cap (B + \mathbf{L})\ ) \\
&= \sum_{X \in \mathbf{L}} \nu\Big(\mathbf{J}_1 \cap [X, I](\mathbf{J}_2 \cap (B + \mathbf{L}))\Big) \\
&= \sum_{X \in \mathbf{L}} \nu\Big([X, I]^{-1}(\mathbf{J}_1) \cap \mathbf{J}_2 \cap (B + \mathbf{L})\Big) \\
&\text{(because } [X, I] \cdot \nu = \nu) \\
&= \nu(\bigcup_{X \in \mathbf{L}} [-X, I](\mathbf{J}_1) \cap \mathbf{J}_2 \cap (B + \mathbf{L})\ ) \\
&= \nu(\mathbf{J}_2 \cap (B + \mathbf{L})) \\
&= n_2(B + \mathbf{L}) \\
&= \rho_*(n_2)(B + \mathbf{L})
\end{aligned}$$

Hence:

$$\rho_*(n_1) = \rho_*(n_2)$$

It follows that σ has invariant meaning, independent of selection of the cross section $\mathbf{J}$ for $\mathbf{L}$.

49° Now we know that each classical crystal ν determines an ordered pair $(\mathbf{L}, \sigma)$:

$$\nu \longrightarrow (\mathbf{L}, \sigma)$$

where $\mathbf{L}$ is a lattice in $\mathbf{R}^3$ and where σ is a nonnegative real valued measure defined on the Borel subsets of the quotient group $\mathbf{\Omega}$. Conversely, each such ordered pair $(\mathbf{L}, \sigma)$ determines a classical crystal ν:

$$(\mathbf{L}, \sigma) \longrightarrow \nu$$

Thus:

$$\nu = n * \delta_{\mathbf{L}}$$

where $\mathbf{J}$ is any cross section for $\mathbf{L}$ and where n is the nonnegative real valued measure defined on $\mathcal{B}$, designed to meet the conditions $supp(n) \subseteq \mathbf{J}$ and $\rho_*(n) = \sigma$. One can easily adapt the computation displayed in the foregoing article to show that ν remains the same though $\mathbf{J}$ be varied.

50° Let us note that the following composition of the foregoing mappings:

$$\nu \longrightarrow (\mathbf{L}, \sigma) \longrightarrow \nu$$

returns each classical crystal ν to itself. That is so essentially by definition. However, the alternative composition:

$$(\mathbf{L}_0, \sigma_0) \longrightarrow \nu \longrightarrow (\mathbf{L}, \sigma)$$

returns an ordered pair $(\mathbf{L}_0, \sigma_0)$ to itself iff:

$$\mathbf{T}_\nu = \mathbf{L}_0$$

In general, we have $\mathbf{L}_0 \subseteq \mathbf{T}_\nu = \mathbf{L}$ and $\sigma = \pi_*(\sigma_0)$, where π is the natural homomorphism carrying $\mathbf{\Omega}_0$ to $\mathbf{\Omega}$:

$$\pi(V + \mathbf{L}_0) = V + \mathbf{L}$$

where V is any position vector in $\mathbf{R}^3$. Given that:

$$(\mathbf{L}_0, \sigma_0) \longrightarrow \nu$$

we contend that $\mathbf{T}_\nu = \mathbf{L}_0$ iff σ_0 meets a certain condition of *minimum translational symmetry*.

51° Thus, for each T in $\mathbf{R}^3$, let τ_T be the *translation* on $\mathbf{\Omega}_0$ defined as follows:

$$\tau_T(V + \mathbf{L}_0) = T + V + \mathbf{L}_0$$

where V is any position vector in $\mathbf{R}^3$. In turn, let $\tau_T \cdot \sigma_0$ be the *transform* of σ_0 by τ_T:

$$\tau_T \cdot \sigma_0 = (\tau_T)_*(\sigma_0)$$

That is, for any B in $\mathcal{B}$:

$$(\tau_T \cdot \sigma_0)(B + \mathbf{L}_0) = \sigma_0(-T + B + \mathbf{L}_0)$$

We contend that, for each T in $\mathbf{R}^3$:

$$\tau_T \cdot \sigma_0 = \sigma_0 \quad \text{iff} \quad T \in \mathbf{T}_\nu$$

To prove the contention, let us introduce a cross section $\mathbf{J}_0$ for $\mathbf{L}_0$ and the restriction n_0 of ν to $\mathbf{J}_0$. Let T be any vector in $\mathbf{R}^3$. Clearly, $\tau_T \rho_0 = \rho_0[T, I]$, so:

$$\tau_T \cdot \sigma_0 = (\rho_0)_*([T, I] \cdot n_0)$$

Moreover:

$$[T, I] \cdot \nu = ([T, I] \cdot n_0) * \delta_{\mathbf{L}_0}$$

Let $\bar{n}_0$ stand for the restriction of ν to the cross section $[T, I](\mathbf{J}_0)$ for $\mathbf{L}_0$. If $\tau_T \cdot \sigma_0 = \sigma_0$ then $[T, I] \cdot n_0 = \bar{n}_0$; therefore $[T, I] \cdot \nu = \bar{n}_0 * \delta_{\mathbf{L}_0} = \nu$. Conversely, if $[T, I] \cdot \nu = \nu$ then $[T, I] \cdot n_0 = \bar{n}_0$; therefore $\tau_T \cdot \sigma_0 = \sigma_0$. Hence, $\tau_T \cdot \sigma_0 = \sigma_0$ iff $T \in \mathbf{L}_\nu$.

52° Of course, τ_T is the identity mapping on Ω_0 iff $T \in \mathbf{L}$.

53° Now we can say that the correspondence:

$$\nu \longleftrightarrow (\mathbf{L}, \sigma)$$

is bijective, provided that σ meets the condition of minimum translational symmetry.

54° Let us digress to describe an interesting instance of classical crystals: the *diamond crystal*. For this crystal, carbon atoms occupy the positions in $\mathbf{R}^3$ defined by the various vectors in the set:

$$\mathbf{K} + \mathbf{L}$$

where:

$$\mathbf{L} = \frac{1}{2} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} (\mathbf{Z}^3)$$

where:

$$S_0 = \frac{1}{4} \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad S_1 = \frac{1}{4} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = S$$

and where:

$$\mathbf{K} = \{S_0, S_1\} = \{O, S\}$$

Presumably, the distributions of electrons at each position in the crystal are identical. Hence, as a first approximation, we can define the global electron distribution for the diamond crystal as follows:

$$\nu = \delta_{\mathbf{K}} * \delta_{\mathbf{L}} = \sum_{k=0}^{1} [S_k, I] \cdot \delta_{\mathbf{L}} = \delta_{\mathbf{L}} + [S, I] \cdot \delta_{\mathbf{L}}$$

55° Clearly, $\delta_{\mathbf{K}}$ is the local electron distribution for ν, relative to the cross section:

$$\mathbf{J} = \frac{1}{2} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} (\mathbf{I})$$

for $\mathbf{L}$. One can easily verify that $\sigma = \rho_*(\delta_{\mathbf{K}})$ meets the condition of minimum translational symmetry, so that $\mathbf{T}_\nu = \mathbf{L}$. However, it is instructive to check the fact directly. Thus, for each T in $\mathbf{R}^3$:

$$[T, I] \cdot (\delta_{\mathbf{L}} + [S, I] \cdot \delta_{\mathbf{L}}) = [T, I] \cdot \delta_{\mathbf{L}} + [T + S, I] \cdot \delta_{\mathbf{L}}$$

Hence, $[T, I] \cdot \nu = \nu$ iff either:

$$T + \mathbf{L} = \mathbf{L} \quad \text{and} \quad T + S + \mathbf{L} = S + \mathbf{L}$$

or:

$$T + \mathbf{L} = S + \mathbf{L} \quad \text{and} \quad T + S + \mathbf{L} = \mathbf{L}$$

For the latter case, we would infer that $2S \in \mathbf{L}$, which is false. We conclude that $[T, I] \cdot \nu = \nu$ iff $T \in \mathbf{L}$. That is, $\mathbf{T}_\nu = \mathbf{L}$.

56° Among the 14 Bravais forms, one refers to $\mathbf{L}$ as the *face centered cubic* lattice. Let us denote by:

$$\mathbf{O}_{\mathbf{L}}$$

the subgroup of $\mathbf{O}$ comprised of all Λ for which $\Lambda(\mathbf{L}) = \mathbf{L}$. One can easily check that:

$$\Lambda(\mathbf{L}) = \mathbf{L} \quad \text{iff} \quad \Lambda(\mathbf{Z}^3) = \mathbf{Z}^3$$

so that $\mathbf{O}_{\mathbf{L}}$ contains 48 members. We know that $\mathbf{\Lambda}_\nu \subseteq \mathbf{O}_{\mathbf{L}}$. We will find that $\mathbf{\Lambda}_\nu = \mathbf{O}_{\mathbf{L}}$. Even so, the final description of $\mathbf{C}_\nu$ yields a surprise.

57° For each $[\bar{T}, \Lambda]$ in $\mathbf{C}$:

$$\begin{aligned} [\bar{T}, \Lambda] \cdot (\delta_{\mathbf{L}} + [S, I] \cdot \delta_{\mathbf{L}}) &= [\bar{T}, I] \cdot ([0, \Lambda] \cdot \delta_{\mathbf{L}} + ([\Lambda(S), I] \cdot ([0, \Lambda]) \cdot \delta_{\mathbf{L}}) \\ &= [\bar{T}, I] \cdot (\delta_{\Lambda(\mathbf{L})} + [\Lambda(S), I] \cdot \delta_{\Lambda(\mathbf{L})}) \\ &= [\bar{T}, I] \cdot \delta_{\Lambda(\mathbf{L})} + [\bar{T} + \Lambda(S), I] \cdot \delta_{\Lambda(\mathbf{L})} \end{aligned}$$

Hence, $[\bar{T}, \Lambda] \cdot \nu = \nu$ iff $\Lambda \in \mathbf{O_L}$ and either:

$$\bar{T} + \mathbf{L} = \mathbf{L} \quad \text{and} \quad \bar{T} + \Lambda(S) + \mathbf{L} = S + \mathbf{L}$$

or:

$$\bar{T} + \mathbf{L} = S + \mathbf{L} \quad \text{and} \quad \bar{T} + \Lambda(S) + \mathbf{L} = \mathbf{L}$$

Moreover, for each Λ in $\mathbf{O_L}$:

$$\Lambda(\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}) = \begin{pmatrix} \Sigma^1 \\ \Sigma^2 \\ \Sigma^3 \end{pmatrix}$$

where each of Σ^1, Σ^2, and Σ^3 equals either -1 or 1. It follows that either $S - \Lambda(S) \in \mathbf{L}$ or $S + \Lambda(S) \in \mathbf{L}$. By these relations, we are led to introduce the partition:

$$\mathbf{O_L} = \mathbf{O_L^0} \ \cup \ (-I)\mathbf{O_L^0}$$

of $\mathbf{O_L}$, where $\mathbf{O_L^0}$ is the subgroup of $\mathbf{O_L}$ defined by the condition:

$$S - \Lambda(S) \in \mathbf{L}$$

and where $(-I)\mathbf{O_L^0}$ is the coset of $\mathbf{O_L^0}$ defined by the condition:

$$S + \Lambda(S) \in \mathbf{L}$$

Of course, the index of $\mathbf{O_L^0}$ in $\mathbf{O_L}$ is 2, so $\mathbf{O_L^0}$ contains 24 members. By inspection, we conclude that the members $[\bar{T}, \Lambda]$ of $\mathbf{C}_\nu$ stand in one or the other of the following forms:

$$[T, \Lambda] \qquad (T \in \mathbf{L}, \ \ \Lambda \in \mathbf{O_L^0})$$

and:

$$[T, I][S, \Lambda] \qquad (T \in \mathbf{L}, \ \ \Lambda \in (-I)\mathbf{O_L^0})$$

In particular:

$$\mathbf{\Lambda}_\nu = \mathbf{O_L}$$

58° By the foregoing analysis, we have shown that the symmetry group $\mathbf{C}_\nu$ of the diamond crystal is an extension of the face centered cubic lattice $\mathbf{L}$ by the full symmetry group $\mathbf{O_L}$ of that lattice:

$$\mathbf{L} \xrightarrow{\theta} \mathbf{C}_\nu \xrightarrow{\pi} \mathbf{O_L}$$

However, $\mathbf{C}_\nu$ is not the simple *symmorphic* case:

$$\mathbf{L} \rtimes \mathbf{O_L}$$

comprised of all $[T, \Lambda]$ in $\mathbf{C}$ of the form:

$$[T, \Lambda] \qquad (T \in \mathbf{L}, \quad \Lambda \in \mathbf{O_L})$$

Rather, it is something "more interesting:" one of the *nonsymmorphic* cases, just described. The group $\mathbf{C}_\nu$ contains symmetries:

$$[\bar{T}, \Lambda] = [\bar{T}, I]\,[O, \Lambda]$$

for which neither $[\bar{T}, I]$ nor $[O, \Lambda]$ lies in $\mathbf{C}_\nu$.

59° By the way, the lattice $\mathbf{M}$ reciprocal to $\mathbf{L}$ is the *body centered cubic* lattice:

$$\mathbf{M} = \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix} (\mathbf{Z}^3)$$

60° Seeking simplicity in the description of classical crystals and in the interpretation of diffraction patterns, crystallographers often violate the condition of minimum translational symmetry. In effect, they employ ordered pairs $(\mathbf{L}_0, \sigma_0)$ for which:

$$(\mathbf{L}_0, \sigma_0) \longrightarrow \nu$$

where $\mathbf{L}_0$ is strictly smaller than $\mathbf{T}_\nu$ but simpler in form. They recover the translational symmetries in $\mathbf{T}_\nu \backslash \mathbf{L}_0$ from the translational symmetries of σ_0.

61° Let us illustrate the practice just described, by means of the diamond crystal. We have described the global electron distribution ν for the diamond crystal as follows:

$$\nu = \delta_{\mathbf{K}} * \delta_{\mathbf{L}}$$

where $\mathbf{L}$ is the face centered cubic lattice:

$$\mathbf{L} = \frac{1}{2} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} (\mathbf{Z}^3)$$

where:

$$S_0 = \frac{1}{4} \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad S_1 = \frac{1}{4} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

and where:

$$\mathbf{K} = \{S_0, S_1\}$$

We have noted that $\sigma = \rho_*(\delta_{\mathbf{K}})$ meets the condition of minimum translational symmetry and we have verified that $\mathbf{T}_\nu = \mathbf{L}$. Now, however, let us replace $\mathbf{L}$ by the strictly smaller *simple cubic* lattice $\mathbf{Z}^3$. Of course:

$$\mathbf{L} = \bigcup_{j=0}^{3} (F_j + \mathbf{Z}^3)$$

where:

$$F_0 = \frac{1}{2}\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad F_1 = \frac{1}{2}\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \quad F_2 = \frac{1}{2}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad F_3 = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$$

In turn, let us replace $\mathbf{K}$ by the strictly larger array $\mathbf{Y}$:

$$\mathbf{Y} = \bigcup_{j=0}^{3} \bigcup_{k=0}^{1} \{F_j + S_k\}$$

See Figure 2. Clearly, $\mathbf{I}$ is a cross section for $\mathbf{Z}^3$, $\mathbf{Y} \subseteq \mathbf{I}$, the restriction of ν to $\mathbf{I}$ is $\delta_{\mathbf{Y}}$, and:

$$\nu = \delta_{\mathbf{Y}} * \delta_{\mathbf{Z}^3}$$

Let ρ_0 be the natural homomorphism carrying $\mathbf{R}^3$ to $\mathbf{\Omega}_0 = \mathbf{R}^3/\mathbf{Z}^3 = \mathbf{T}^3$. Let $\sigma_0 = (\rho_0)_*(\delta_{\mathbf{Y}})$. By design:

$$(\mathbf{Z}^3, \sigma_0) \longrightarrow \nu \longrightarrow (\mathbf{L}, \sigma)$$

We can recover the translational symmetries in $\mathbf{L}\backslash\mathbf{Z}^3$ from the translational symmetries for σ_0, by verifying that, for any T in $\mathbf{R}^3$, $\tau_T \cdot \sigma_0 = \sigma_0$ iff there is some j $(0 \leq j \leq 3)$ such that:

$$T \in F_j + \mathbf{Z}^3$$

62° The following Figure suggests the disposition of $\mathbf{Y}$ as a subset of the cube $\mathbf{I}$:

Figure 2

The Figure shows the base for $\mathbf{I}$ in the $(1, 2)$-coordinate plane. The points in $\mathbf{Y}$ represented by white disks have third coordinate 0; by white squares, 1/4; by black disks, 1/2; by black squares, 3/4.

63° For a second example, let us describe, briefly, the *cesium chloride* crystal. For this crystal, chlorine atoms occupy the positions in $\mathbf{R}^3$ defined by the various vectors in the set:

$$\mathbf{Z}^3$$

while cesium atoms occupy the positions in $\mathbf{R}^3$ defined by the various vectors in the set:

$$\{S\} + \mathbf{Z}^3$$

where:

$$S = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

As a first approximation, we can define the global electron distribution for the cesium chloride crystal as follows:

$$\nu = (a\delta_{\{0\}} + b\delta_{\{S\}}) * \delta_{\mathbf{Z}^3}$$

where a and b are distinct positive real numbers. One can readily verify that:

$$\mathbf{T}_\nu = \mathbf{Z}^3 \quad \text{and} \quad \mathbf{\Lambda}_\nu = \mathbf{O}_{\mathbf{Z}^3}$$

and that $\mathbf{C}_\nu$ is the symmorphic case:

$$\mathbf{C}_\nu = \mathbf{Z}^3 \leftthreetimes \mathbf{O}_{\mathbf{Z}^3}$$

6 Fourier Transforms

64° Crystallographers study the structure of classical crystals not by direct but by indirect methods. They gather data from the diffraction patterns produced as the crystals interact with electromagnetic fields. By a formal analysis of such interactions, they describe the relation between classical crystals and diffraction patterns in terms of the relation between global electron distributions ν and Fourier Transforms $\hat{\nu}$. However, their procedures for recovering the structure of classical crystals from the structure of diffraction patterns are rendered problematic, but all the more interesting by the fact that data gathered from the patterns yield not the complex values of $\hat{\nu}$ but only their moduli.

65° Let us review the definition and the fundamental properties of the Fourier Transform. Thus, let f be any complex valued smooth function defined on $\mathbf{R}^3$. One says that f is *rapidly decreasing* iff f and all its partial derivatives are tempered. Let $\mathbf{F}$ stand for the family of all such functions.

66° For each f in $\mathbf{F}$, one defines the *Fourier Transform* $\hat{f}$ of f as follows:

$$\hat{f}(Y) = \int_{\mathbf{R}^3} exp(-2\pi i\, X \bullet Y) f(X) \lambda(dX)$$

where λ is Lebesgue measure defined on $\mathcal{B}$ and where Y is any wave vector in the reciprocal space $\mathbf{R}^3$. One finds that $\hat{f}$ is rapidly decreasing and that:

$$f(X) = \int_{\mathbf{R}^3} exp(+2\pi i\, X \bullet Y) \hat{f}(Y) \lambda(dY)$$

where X is any position vector in the real space $\mathbf{R}^3$.

67° Let us note that the functions f and $\hat{f}$ are related by the celebrated *Poisson Summation Formula*:

$$\sum_{U \in \mathbf{Z}^3} f(U) \;=\; \sum_{V \in \mathbf{Z}^3} \hat{f}(V)$$

68° Let us adapt the foregoing formula to an arbitrary pair $\mathbf{L}$ and $\mathbf{M}$ of mutually reciprocal lattices. Thus, let $\mathcal{L}$ be an invertible linear mapping carrying $\mathbf{R}^3$ to itself for which $\mathbf{L} = \mathcal{L}(\mathbf{Z}^3)$ and $\mathbf{M} = (\mathcal{L}^{-1})^*(\mathbf{Z}^3)$. For each f in $\mathbf{F}$, let $g = f \cdot \mathcal{L}$. For each V in $\mathbf{R}^3$:

$$\begin{aligned} \hat{g}(V) &= \int_{\mathbf{R}^3} exp(-2\pi i\, U \bullet V) g(U) \nu(dU) \\ &= \frac{1}{|det(\mathcal{L})|} \int_{\mathbf{R}^3} exp(-2\pi i\, \mathcal{L}^{-1}(X) \bullet V) f(X) \nu(dX) \end{aligned}$$

Hence:

$$\hat{g}(V) = \frac{1}{|det(\mathcal{L})|}\, \hat{f}((\mathcal{L}^{-1})^*(V))$$

and therefore:

$$\sum_{X \in \mathbf{L}} f(X) \;=\; \sum_{U \in \mathbf{Z}^3} g(U) = \sum_{V \in \mathbf{Z}^3} \hat{g}(V) = \frac{1}{|\mathbf{L}|} \sum_{Y \in \mathbf{M}} \hat{f}(Y)$$

where $|\mathbf{L}| = |det(\mathcal{L})|$. One can easily show that $|\mathbf{L}|$ remains the same though $\mathcal{L}$ be varied. Finally, we present the general Poisson Summation Formula:

$$\sqrt{|\mathbf{L}|} \sum_{X \in \mathbf{L}} f(X) = \sqrt{|\mathbf{M}|} \sum_{Y \in \mathbf{M}} \hat{f}(Y)$$

69° For each tempered measure μ defined on $\mathcal{B}$, one defines the *Fourier Transform* $\hat{\mu}$ of μ as follows:

$$\hat{\mu}(f) = \int_{\mathbf{R}^3} \hat{f}(V)\mu(dV)$$

where f is any function in $\mathbf{F}$. We hasten to note that, so defined, $\hat{\mu}$ is simply a linear functional on $\mathbf{F}$. However, we contend that if μ coincides with a classical crystal ν then in fact $\hat{\mu}$ can be identified with a tempered measure.

70° Let us prove the foregoing contention. Let ν be a classical crystal. Let $\mathbf{L} = \mathbf{T}_\nu$, let $\mathbf{J}$ be a cross section for $\mathbf{L}$, and let n be the restriction of ν to $\mathbf{J}$. As usual, we find:

$$\nu = n * \delta_{\mathbf{L}}$$

Let $\mathbf{\Omega} = \mathbf{R}^3/\mathbf{L}$ and let ρ be the natural homomorphism carrying $\mathbf{R}^3$ to $\mathbf{\Omega}$. Let $\sigma = \rho_*(n)$. As noted earlier, we find:

$$\nu \longrightarrow (\mathbf{L}, \sigma) \longrightarrow \nu$$

Let $\mathbf{M}$ be the lattice reciprocal to $\mathbf{L}$. For each Y in $\mathbf{R}^3$, $Y \in \mathbf{M}$ iff, for each X in $\mathbf{L}$:

$$exp(+2\pi i\, X \bullet Y) = 1$$

Hence, we can identify $\mathbf{M}$ with the dual group $\mathbf{\Omega}^*$ for $\mathbf{\Omega}$. One should note that:

$$\kappa = \frac{1}{\lambda(\mathbf{J})}\rho_*(\lambda{\downarrow}\mathbf{J})$$

is the normalized haar measure on $\mathbf{\Omega}$, where ρ is the canonical mapping carrying $\mathbf{R}^3$ to $\mathbf{\Omega} = \mathbf{R}^3/\mathbf{L}$. That said, we can introduce the (normalized) *Fourier Transform* $\hat{\sigma}$ of σ as follows:

$$\begin{aligned}\hat{\sigma}(Y) =& \frac{1}{\lambda(\mathbf{J})}\int_{\mathbf{\Omega}} \langle\!\langle\, X + \mathbf{L}, Y \,\rangle\!\rangle^* \sigma(d(X + \mathbf{L})) \\ =& \frac{1}{\lambda(\mathbf{J})}\int_{\mathbf{J}} exp(-2\pi i\, X \bullet Y) n(dX)\end{aligned}$$

where Y is any reciprocal vector in $\mathbf{M}$. Of course, $\lambda(\mathbf{J}) = |\mathbf{L}|$.

71° Finally, let us introduce the complex valued measure $\hat{\sigma} \cdot \delta_{\mathbf{M}}$ defined on $\mathcal{B}$ such that, for each Y in $\mathbf{M}$:

$$(\hat{\sigma} \cdot \delta_{\mathbf{M}})(\{Y\}) = \hat{\sigma}(Y)$$

while, for any B in $\mathcal{B}$, if $B \cap \mathbf{M} = \emptyset$ then $(\hat{\sigma} \cdot \delta_{\mathbf{M}})(B) = 0$. Obviously, $\hat{\sigma} \cdot \delta_{\mathbf{M}}$ is tempered and, for each f in $\mathbf{F}$:

$$\int_{\mathbf{R}^3} f(Y)(\hat{\sigma} \cdot \delta_{\mathbf{M}})(dY) = \sum_{Y \in \mathbf{M}} \hat{\sigma}(Y) f(Y)$$

We contend now that:

$$\hat{\nu} = \hat{\sigma} \cdot \delta_{\mathbf{M}}$$

That is, for each f in $\mathbf{F}$:

$$\hat{\nu}(f) = \int_{\mathbf{R}^3} f(Y)(\hat{\sigma} \cdot \delta_{\mathbf{M}})(dY)$$

To prove the contention, we compute:

$$\begin{aligned}
\hat{\nu}(f) &= \int_{\mathbf{R}^3} \hat{f}(V)\nu(dV) \\
&= \int_{\mathbf{R}^3} \int_{\mathbf{J}} \hat{f}(W + X) n(dW) \delta_{\mathbf{L}}(dX) \\
&= \int_{\mathbf{R}^3} \int_{\mathbf{J}} \int_{\mathbf{R}^3} exp(-2\pi i (W + X) \bullet Y) f(Y) \lambda(dY) n(dW) \delta_{\mathbf{L}}(dX) \\
&= |\mathbf{L}| \int_{\mathbf{R}^3} \int_{\mathbf{R}^3} exp(-2\pi i X \bullet Y) \hat{\sigma}(Y) f(Y) \lambda(dY) \delta_{\mathbf{L}}(dX) \\
&= |\mathbf{L}| \int_{\mathbf{R}^3} \hat{g}(X) \delta_{\mathbf{L}}(dX) \qquad (\text{where } \; g = \hat{\sigma}\, f) \\
&= |\mathbf{L}| \sum_{X \in \mathbf{L}} \hat{g}(X) \\
&= \sum_{Y \in \mathbf{M}} g(Y) \qquad (\text{because } \; |\mathbf{L}||\mathbf{M}| = 1, \; 68^\circ) \\
&= \sum_{Y \in \mathbf{M}} \hat{\sigma}(Y) f(Y) \\
&= \int_{\mathbf{R}^3} f(Y)(\hat{\sigma} \cdot \delta_{\mathbf{M}})(dY)
\end{aligned}$$

72° For the case in which:

$$n = \delta_{\{O\}}$$

we find a reformulation of the Poisson Summation Formula:

$$\sqrt{|\mathbf{L}|}\, \hat{\delta}_{\mathbf{L}} = \sqrt{|\mathbf{M}|}\, \delta_{\mathbf{M}}$$

73° Now let us attempt to explain the physical relation between classical crystals and the corresponding diffraction patterns, in terms of the mathematical relation between tempered nonnegative real valued measures and the corresponding Fourier Transforms. We will apply the formalism of Scattering Theory, treating the interaction between classical crystals and electromagnetic fields, roughly, as a problem of elastic scattering.

74° ∘
∘
∘
∘
∘
∘
∘

7 Generalized Crystals

75° Let ν be a classical crystal. The symmetry group $\mathbf{C}_\nu$ for ν figures in a short exact sequence, as follows:

$$\mathbf{L} \xrightarrow{\theta} \mathbf{C}_\nu \xrightarrow{\phi} \mathbf{\Gamma}$$

where $\mathbf{L} = \mathbf{T}_\nu$ is the lattice and where $\mathbf{\Gamma} = \mathbf{\Lambda}_\nu$ is the point group for ν. Let $\mathbf{\Omega}$ be the compact Abelian quotient group:

$$\mathbf{\Omega} = \mathbf{R}^3/\mathbf{L}$$

and let ρ be the natural homomorphism carrying $\mathbf{R}^3$ to $\mathbf{\Omega}$. We can identify ν with the ordered pair:

$$(\mathbf{L}, \sigma)$$

where σ is the nonnegative real valued measure on $\mathbf{\Omega}$, defined by introducing a cross section $\mathbf{J}$ of $\mathbf{L}$ and, in turn, the restriction n of ν to $\mathbf{J}$, then projecting n to $\mathbf{\Omega}$ by ρ:

$$\sigma = \rho_*(n)$$

The measure σ remains the same though $\mathbf{J}$ be varied. In turn, we can identify the ordered pair $(\mathbf{L}, \sigma)$ with the ordered pair:

$$(\mathbf{M}, \hat{\sigma})$$

where $\mathbf{M}$ is the lattice reciprocal to $\mathbf{L}$ and where $\hat{\sigma}$ is the (normalized) Fourier Transform of σ. Of course, $\mathbf{M}$ coincides with the discrete Abelian group $\mathbf{\Omega}^*$ dual to $\mathbf{\Omega}$ and $\hat{\sigma}$ is a function defined on $\mathbf{M}$.

76° We can display the natural pairing between $\mathbf{\Omega} = \mathbf{R}^3/\mathbf{L}$ and $\mathbf{\Omega}^* = \mathbf{M}$ as follows:

$$\langle\!\langle\, V + \mathbf{L}, Y \,\rangle\!\rangle = exp(2\pi i\, V \bullet Y)$$

where V is any position vector in $\mathbf{R}^3$ and where Y is any reciprocal vector in $\mathbf{M}$.

77° Let h be a complex valued function defined on $\mathbf{M}$. One says that h is *positive definite* iff, for any positive integer m and for any reciprocal vectors:

$$Y_1, Y_2, \ \ldots\ , Y_m$$

in $\mathbf{M}$, the m by m matrix:

$$\{h(Y_k - Y_\ell)\} \qquad (1 \leq k \leq m,\ 1 \leq \ell \leq m)$$

is self adjoint and nonnegative. We can apply the Theorem of S. Bochner to characterize the functions $\hat{\sigma}$ as continuous positive definite functions defined on $\mathbf{M}$.

78° Let us emphasize that σ meets the condition of minimum translational symmetry. For $\hat{\sigma}$, this condition means that $supp(\hat{\sigma})$ generates $\mathbf{M}$.

79° Let us refer to the ordered pair $(\mathbf{M}, \hat{\sigma})$ as the *dual form* for ν.

80° For classical crystals, we have introduced the relations of congruence and equivalence. See articles 41° and 42°. Let us now seek expressions for these relations in terms of dual forms.

81° As usual, let $\mathbf{A}$ be the group of all affine mappings carrying $\mathbf{R}^3$ to itself, and let $\mathbf{C}$ be the subgroup of $\mathbf{A}$ comprised of all Cartesian mappings carrying $\mathbf{R}^3$ to itself. Let $\mathbf{N}$ be the set of all classical crystals. With reference to article 36°, let us introduce the action of $\mathbf{A}$ on $\mathbf{N}$, as follows:

$$([T, \Lambda],\, \nu) \longrightarrow [T, \Lambda] \cdot \nu = [T, \Lambda]_*(\nu)$$

Of course, we obtain by restriction the action of $\mathbf{C}$ on $\mathbf{N}$. For any ν' and ν'' in $\mathbf{N}$, ν' and ν'' are congruent iff they lie in the same orbit in $\mathbf{N}$ under $\mathbf{C}^+$. They are equivalent iff their stabilizers $\mathbf{C}_{\nu'}$ and $\mathbf{C}_{\nu''}$ in $\mathbf{C}$ are conjugate in $\mathbf{A}^+$.

82° Now let $\mathbf{\Sigma}$ be the set of all ordered pairs $(\mathbf{L}, \sigma)$, where $\mathbf{L}$ is a lattice in the real space $\mathbf{R}^3$ and where σ is a nonnegative real valued measure defined on the compact Abelian quotient group $\mathbf{\Omega} = \mathbf{R}^3/\mathbf{L}$, which meets the condition

of minimum translational symmetry. For any $[T, \Lambda]$ in $\mathbf{A}$ and for any $(\mathbf{L}', \sigma')$ and $(\mathbf{L}'', \sigma'')$ in $\mathbf{\Sigma}$, let us write:

$$(\mathbf{L}'', \sigma'') = [T, \Lambda] \cdot (\mathbf{L}', \sigma')$$

to express the conditions that:

$$\mathbf{L}'' = \Lambda(\mathbf{L}')$$
$$\sigma'' = (\tau_T \hat{\Lambda})_*(\sigma')$$

where $\hat{\Lambda}$ is the isomorphism carrying $\mathbf{\Omega}'$ to $\mathbf{\Omega}''$ defined by Λ and where τ_T is the translation carrying $\mathbf{\Omega}''$ to itself defined by T. To be clear, let us note that:

$$\hat{\Lambda}(V_1 + \mathbf{L}') = \Lambda(V_1) + \mathbf{L}''$$
$$\tau_T(V_2 + \mathbf{L}'') = T + V_2 + \mathbf{L}''$$

where V_1 and V_2 are any position vectors in $\mathbf{R}^3$. Clearly, these relations define an action of $\mathbf{A}$ on $\mathbf{\Sigma}$ and, by restriction, an action of $\mathbf{C}$ on $\mathbf{\Sigma}$.

83° The bijective mapping:

$$\nu \longrightarrow (\mathbf{L}, \sigma)$$

carrying $\mathbf{N}$ to $\mathbf{\Sigma}$ intertwines the actions of $\mathbf{A}$. That is, for any $[T, \Lambda]$ in $\mathbf{A}$ and for any ν' and ν'' in $\mathbf{N}$, $\nu'' = [T, \Lambda] \cdot \nu'$ iff $(\mathbf{L}'', \sigma'') = [T, \Lambda] \cdot (\mathbf{L}', \sigma')$, where $(\mathbf{L}', \sigma')$ and $(\mathbf{L}'', \sigma'')$ are the ordered pairs in $\mathbf{\Sigma}$ corresponding to ν' and ν''. Of course, this consideration motivated the definition of the action of $\mathbf{A}$ on $\mathbf{\Sigma}$ in the first place.

84° The various mappings:

$$\tau_T \hat{\Lambda}$$

are instances of *affine* mappings carrying $\mathbf{\Omega}'$ to $\mathbf{\Omega}''$: compositions of isomorphisms and translations. In our context, one can easily show that every affine mapping carrying $\mathbf{\Omega}'$ to $\mathbf{\Omega}''$ stands in the foregoing form. Among the affine mappings, the *Cartesian* mappings carrying $\mathbf{\Omega}'$ to $\mathbf{\Omega}''$ are those for which Λ is orthogonal.

85° In turn, let $\hat{\mathbf{\Sigma}}$ be the set of all ordered pairs $(\mathbf{M}, \hat{\sigma})$, where $\mathbf{M}$ is a lattice in the reciprocal space $\mathbf{R}^3$ and where $\hat{\sigma}$ is a positive definite complex valued function defined on $\mathbf{M}$, for which $supp(\hat{\sigma})$ generates $\mathbf{M}$. For any $[T, \Lambda]$ in $\mathbf{A}$ and for any $(\mathbf{M}', \hat{\sigma}')$ and $(\mathbf{M}'', \hat{\sigma}'')$ in $\hat{\mathbf{\Sigma}}$, let us write:

$$(\mathbf{M}'', \hat{\sigma}'') = [T, \Lambda] \cdot (\mathbf{M}', \hat{\sigma}')$$

to express the conditions that:

$$\mathbf{M}'' = (\Lambda^*)^{-1}(\mathbf{M}')$$
$$\hat{\sigma}'' = \frac{1}{|det(\Lambda)|}\rho''(T)^*((\Lambda^*)^{-1} \cdot \hat{\sigma}')$$

where ρ'' is the natural homomorphism carrying $\mathbf{R}^3$ to $\mathbf{\Omega}''$. To be clear, let us note that, for any reciprocal vector Z in $\mathbf{M}''$:

$$((\Lambda^*)^{-1} \cdot \hat{\sigma}')(Z) = \hat{\sigma}'(\Lambda^*(Z))$$
$$\rho''(T)^*(Z) = \langle\!\langle\, T + \mathbf{L}'', Z \,\rangle\!\rangle^*$$

Replacing Z by the reciprocal vector $Y = \Lambda^*(Z)$ in $\mathbf{M}'$, we find that:

$$\hat{\sigma}''((\Lambda^*)^{-1}(Y)) = \frac{1}{|det(\Lambda)|}\langle\!\langle\, \Lambda^{-1}(T) + \mathbf{L}', Y \,\rangle\!\rangle^* \hat{\sigma}'(Y)$$

Of course, $T + \mathbf{L}'' \in \mathbf{\Omega}'' = \mathbf{R}^3/\mathbf{L}''$. Clearly, these relations define an action of $\mathbf{A}$ on $\hat{\mathbf{\Sigma}}$ and, by restriction, an action of $\mathbf{C}$ on $\hat{\mathbf{\Sigma}}$.

86° For any $[T, \Lambda]$ in $\mathbf{C}$, the foregoing relations take the following simpler form:

$$\mathbf{M}'' = \Lambda(\mathbf{M}')$$
$$\hat{\sigma}'' = \rho''(T)^*(\Lambda \cdot \hat{\sigma}')$$

and:

$$(\Lambda \cdot \hat{\sigma}')(Z) = \hat{\sigma}'(\Lambda^{-1}(Z))$$
$$\rho''(T)^*(Z) = \langle\!\langle\, T + \mathbf{L}'', Z \,\rangle\!\rangle^*$$

so that:

$$\hat{\sigma}''(\Lambda(Y)) = \langle\!\langle\, \Lambda^{-1}(T) + \mathbf{L}', Y \,\rangle\!\rangle^* \hat{\sigma}'(Y)$$

87° The bijective mapping:

$$(\mathbf{L}, \sigma) \longrightarrow (\mathbf{M}, \hat{\sigma})$$

carrying $\mathbf{\Sigma}$ to $\hat{\mathbf{\Sigma}}$ intertwines the actions of $\mathbf{A}$. That is, for any $[T, \Lambda]$ in $\mathbf{A}$ and for any $(\mathbf{L}', \sigma')$ and $(\mathbf{L}'', \sigma'')$ in $\mathbf{\Sigma}$:

$$(\mathbf{L}'', \sigma'') = [T, \Lambda] \cdot (\mathbf{L}', \sigma') \quad \text{iff} \quad (\mathbf{M}'', \hat{\sigma}'') = [T, \Lambda] \cdot (\mathbf{M}', \hat{\sigma}')$$

where $(\mathbf{M}', \hat{\sigma}')$ and $(\mathbf{M}'', \hat{\sigma}'')$ are the ordered pairs in $\hat{\mathbf{\Sigma}}$ corresponding to $(\mathbf{L}', \sigma')$ and $(\mathbf{L}'', \sigma'')$. Let us prove that it is so. Obviously, $\Lambda(\mathbf{L}') = \mathbf{L}''$ iff $\Lambda^*(\mathbf{M}'') = \mathbf{M}'$. For each V in $\mathbf{R}^3$, let $W = T + \Lambda(V)$, so that:

$$(\tau_T \hat{\Lambda})(V + \mathbf{L}') = W + \mathbf{L}''$$

For each Y in $\mathbf{M}''$, we have:

$$\hat{\sigma}''(Y) = \frac{1}{|\mathbf{L}''|}\int_{\mathbf{\Omega}''} \langle\!\langle\, W + \mathbf{L}'', Y \,\rangle\!\rangle^* \sigma''(d(W + \mathbf{L}''))$$

and:

$$\begin{aligned}
&\frac{1}{|det(\Lambda)|}\langle\!\langle\, T + \mathbf{L}'', Y \,\rangle\!\rangle^* \hat{\sigma}'(\Lambda^*(Y)) \\
&\qquad = \frac{1}{|det(\Lambda)|}\langle\!\langle\, T + \mathbf{L}'', Y \,\rangle\!\rangle^* \frac{1}{|\mathbf{L}'|}\int_{\mathbf{\Omega}'} \langle\!\langle\, V + \mathbf{L}', \Lambda^*(Y) \,\rangle\!\rangle^* \sigma'(d(V + \mathbf{L}')) \\
&\qquad = \frac{1}{|\mathbf{L}''|}\int_{\mathbf{\Omega}'} \langle\!\langle\, W + \mathbf{L}'', Y \,\rangle\!\rangle^* \sigma''(d(W + \mathbf{L}''))
\end{aligned}$$

because:

$$|det(\Lambda)| = \frac{|\mathbf{L}''|}{|\mathbf{L}'|}$$

Hence:

$$\sigma'' = (\tau_T \hat{\Lambda})_*(\sigma') \quad \text{iff} \quad \hat{\sigma}'' = \frac{1}{|det(\Lambda)|}\rho''(T)^*((\Lambda^*)^{-1} \cdot \hat{\sigma}')$$

Of course, this consideration motivated the definition of the action of $\mathbf{A}$ on $\hat{\mathbf{\Sigma}}$ in the first place.

88° Let us review our position. We have described classical crystals in three different but equivalent ways:

$$\nu, \quad (\mathbf{L}, \sigma), \quad (\mathbf{M}, \hat{\sigma})$$

yielding sets $\mathbf{N}$, $\mathbf{\Sigma}$, and $\hat{\mathbf{\Sigma}}$ in bijective correspondence. For these sets, we have described the natural actions of the affine group $\mathbf{A}$, and we have noted/verified that these actions are, in the obvious sense, equivalent:

$$A.\nu' = \nu'' \iff A.(\mathbf{L}', \sigma') = (\mathbf{L}'', \sigma'') \iff A.(\mathbf{M}', \hat{\sigma}') = (\mathbf{M}'', \hat{\sigma}'')$$

where $A = [T, L]$ is any affine transformation, where ν' and ν'' are any classical crystals, where $(\mathbf{L}', \sigma')$ and $(\mathbf{L}'', \sigma'')$ are the corresponding component forms in real space, and where $(\mathbf{M}', \hat{\sigma}')$ and $(\mathbf{M}'', \hat{\sigma}'')$ are the corresponding component forms in reciprocal space.

89° Cocycle Identity?

8 SuperSpace

9 Computations