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SPACE–TIME SYMMETRIES OF CRYSTAL DIFFRACTION

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Synopsis

An electromagnetic four-potential describing the superposition of a crystal and an electromagnetic plane wave is shown to be invariant with respect to a four-dimensional lattice translation group in space–time. Diffraction (in the kinematical approximation) leaves this group unchanged and this property is equivalent with Bragg's law.

Crystallographic groups in the Minkowskian and Galilean space–time are special cases of relativistic symmetry groups that have been investigated by us recently; some mathematical results have already been published[1,2,3,4]. In this paper an example of physical systems having such symmetries is given.

The superposition of a plane wave and a crystal is invariant with respect to a four-dimensional discrete space–time translation group. Using this property, an analogue of the Bloch theorem has been derived for the case of an electron in the presence of a crystal potential and a monochromatic radiation field[5]). Here another aspect of this space–time symmetry is discussed.

It is shown that the translation group considered above is still a symmetry group of the system even if one takes into account the possible diffraction of the incident plane wave by the crystal (at least in the kinematical approximation). More than that, the Bragg law is equivalent to the requirement that the (elastic) diffraction conserves this symmetry. Actually this lattice translation group is in general not the largest subgroup of the inhomogeneous Lorentz group that is conserved, but in this paper the considerations are restricted to translational symmetries.

The concepts are here discussed for the case of X-ray diffraction; it is clear, however, that they equally well apply to the diffraction of free electrons or of phonons[6]). If other symmetry elements, such as rotations and reflections, are considered, then one has to distinguish between these various cases.

Let the crystal be given by an electrostatic potential $V(\boldsymbol{x})$ invariant with respect to a crystallographic space group G having a discrete translation subgroup U that generates a lattice Γ with basis vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, $\boldsymbol{a}_3$. The most general expression for $V(\boldsymbol{x})$ then is:

$$V(\boldsymbol{x}) = \sum_{\boldsymbol{k}\in\Gamma^*} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\tilde{V}(\boldsymbol{k}) \tag{1}$$

where Γ^* is the lattice generated by the reciprocal basis vectors $\boldsymbol{a}_1^*$, $\boldsymbol{a}_2^*$, $\boldsymbol{a}_3^*$ defined by:

$$\boldsymbol{a}_i\cdot\boldsymbol{a}_k^* = 2\pi\delta_{ik}; \qquad i, k = 1, 2, 3. \tag{2}$$

A transverse electromagnetic wave propagating in the direction $\boldsymbol{h}$ can be obtained from the vector potential:

$$\boldsymbol{A}(\boldsymbol{x}, t) = \boldsymbol{A}\,\mathrm{e}^{\mathrm{i}(\boldsymbol{h}\boldsymbol{x}-\omega t)}, \tag{3}$$

where $\|\boldsymbol{h}\|^2 = (2\pi/\lambda)^2 = (\omega/c)^2$ and $\boldsymbol{A}$ is a constant vector orthogonal to $\boldsymbol{h}$. Consider now the Minkowskian space–time with respect to the orthonormal basis vectors e_1, e_2, e_3, e_4 of the inertial frame in which the crystal is at rest and with metric tensor $e_i\cdot e_j = g_{ij}$ where $g_{11} = g_{22} = g_{33} = -g_{44} = 1$. The superposition of the crystal potential (1) with the plane wave potential (3) gives rise to the electromagnetic four-potential

$$\Phi^j(x) = (A^1(x), A^2(x), A^3(x), V(x)), \qquad x = (\boldsymbol{x}, ct). \tag{4}$$

Note that this potential is of the form:

$$\Phi^j(x) = \sum_{k\in\Lambda_h^*} \mathrm{e}^{\mathrm{i}k\cdot x}\,\tilde{\Phi}^j(k), \qquad j = 1, 2, 3, 4, \tag{5}$$

where Λ_h^* is the four-dimensional lattice generated by Γ^* of eq. (1) and the four-vector of the incident radiation: $h = (\boldsymbol{h}, \omega/c)$. Relation (5) shows that the potential $\Phi^j(x)$, and hence also the electromagnetic field obtained from the superposition of a static crystal with an electromagnetic plane wave, are both invariant with respect to the four-dimensional discrete translation group T_h. This is the group that also leaves invariant the lattice Λ_h defined (in the Minkowskian space) as the reciprocal lattice of Λ_h^*.

An easy calculation shows that if the space component of h is:

$$\boldsymbol{h} = h_1\boldsymbol{a}_1^* + h_2\boldsymbol{a}_2^* + h_3\boldsymbol{a}_3^*, \tag{6}$$

then the set of vectors:

$$\begin{aligned} b_1 &= (\boldsymbol{a}_1, h_1\lambda),\\ b_2 &= (\boldsymbol{a}_2, h_2\lambda),\\ b_3 &= (\boldsymbol{a}_3, h_3\lambda),\\ b_4 &= (0, -\lambda), \end{aligned} \tag{7}$$

forms the basis of Λ_h that is reciprocal to $\{(\boldsymbol{a}_1^*, 0), (\boldsymbol{a}_2^*, 0), (\boldsymbol{a}_3^*, 0), h\}$. The Bragg condition for a diffracted ray $h' = (\boldsymbol{h}', \omega'/c)$ in the elastic case $(\omega' = \omega)$ is expressible in terms of the Laue equation (see for example ref. 7):

$$h' - h = (\boldsymbol{h}' - \boldsymbol{h}, 0) \qquad \text{with} \qquad \boldsymbol{h}' - \boldsymbol{h} \in \Gamma^*. \tag{8}$$

This equation is equivalent to the condition:

$$h' \in \Lambda_{h'}^* \qquad (\text{for} \qquad h'^4 = h^4 = \omega/c). \tag{9}$$

If one considers the lattice $\Lambda_{h'}^*$ obtained as above from the superposition of the given crystal potential with the diffracted wave h', or the corresponding translation group $T_{h'}$, then relation (9) is equivalent to the following ones:

$$\Lambda_h = \Lambda_{h'}, \qquad \text{or} \qquad T_h = T_{h'} \qquad (\text{for } h'^4 = h^4), \tag{10}$$

which simply express the conservation of translational space–time symmetry in the Bragg diffraction. T_h is therefore the translational symmetry group of crystal diffraction. This symmetry group depends only on the crystal, on the incident radiation and on the relative orientation of both, but not (within the kinematical approximation) on the diffracted rays. In proving this result we have not really made use of the Minkowskian metric. And, in fact, one can easily show that the same result is obtained for the case of Galilean space–time. In particular, the group T_h is exactly the same in the Minkowskian and in the Galilean case.

The results of further investigation concerning larger space–time groups having these same properties will be published elsewhere.

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