On The Nature of Group Theory and Condensed Matter Physics

Freddy Alexis Cisneros *December 5, 2017*

This essay addresses an application of Group Theory to the field of Condensed Matter Physics (CMP), primarily to the subject of space groups, point groups, and Bloch's Theorem.

Symmetric Groups of a Crystal

A crystal lattice is a periodic array of atoms which make up the crystal. Often due to the dimensions of the crystal one applies the periodic boundary condition to the lattice since the number of atoms that make up the crystal is on the order of Avagadro's number 10^{23}, the lattice can therefore by approximated as an infinite lattice. Much of the physics that one derives from this approximation is in agreement with experiment when measurements are carried out in the bulk of the material (away from the edges). Because of this periodicity we consider the crystal to be invariant under the following translation,

$$\boldsymbol{r} \rightarrow T(\boldsymbol{l})\boldsymbol{r} = \boldsymbol{r} + \boldsymbol{l}, \tag{1}$$

where $\boldsymbol{l}$ is called the crystal lattice vector and is defined as,

$$\boldsymbol{l} = \boldsymbol{a}_1 l_1 + \boldsymbol{a}_2 l_2 + \boldsymbol{a}_3 l_3, \tag{2}$$

where $l_1, l_2, l_3 \in \mathbb{Z}$, and $\boldsymbol{a}_i$ is a lattice basis vector. Multiplication of two translation's $T(\boldsymbol{l}_i) \cdot T(\boldsymbol{l}_j)$ is defined to be the sum of two crystal lattice vectors, $\boldsymbol{l}_i + \boldsymbol{l}_j$. From this you can easily see the set of all translations $T(\boldsymbol{l})$ which preserve crystal invariance, forms an Abelian group $\mathcal{T}$. This corresponds to a group of translations in the crystal in which the environment of the lattice point $\boldsymbol{r}_1$ (after the translation) looks identical to the environment of the lattice point $\boldsymbol{r}_0$ (before the translation).

In addition to the translational symmetry defined in Eq. 1, a crystal lattice may posses invariance under other symmetric operations which are combinations of spatial inversion, translational, and rotational operations. We will denote this second symmetric operator as $g(R, \boldsymbol{\alpha})$, which acts on $\boldsymbol{r}$ as follows,

$$\boldsymbol{r} \rightarrow g(R, \boldsymbol{\alpha})\boldsymbol{r} = R\boldsymbol{r} + \boldsymbol{\alpha}, \text{ where } R \in O(3), \tag{3}$$

and $\boldsymbol{\alpha}$ is a translation which does not necessarily have to be a crystal lattice vector $\boldsymbol{l}$. From Eq. 3 we see that if $\boldsymbol{\alpha} = 0$ then $g(R, 0) = R$ corresponding to a proper or improper rotation which preserves the origin $\boldsymbol{r}$. If on the other hand $\boldsymbol{\alpha} \neq 0$ and $R = E$ (E being the 3×3 identity matrix) then $\boldsymbol{\alpha}$ must be a crystal lattice vector in order for the crystal to be invariant under the operation defined in Eq. 3 with $g(R, \boldsymbol{\alpha}) = g(E, \boldsymbol{\alpha})$. The multiplication of two symmetry operators $g(R, \boldsymbol{\alpha})$ is defined as follows,

$$\begin{aligned} g(R, \boldsymbol{\alpha})g(R', \boldsymbol{\beta})\boldsymbol{r} &= g(R, \boldsymbol{\alpha})\{R'\boldsymbol{r} + \boldsymbol{\beta}\} \\ &= RR'\boldsymbol{r} + \boldsymbol{\alpha} + R\boldsymbol{\beta} \\ &= (RR')\boldsymbol{r} + (\boldsymbol{\alpha} + R\boldsymbol{\beta}), \end{aligned}$$

from which we see that,

$$g(R, \boldsymbol{\alpha})g(R', \boldsymbol{\beta}) = g(RR', \boldsymbol{\alpha} + R\boldsymbol{\beta}). \tag{4}$$

The inverse of $g(R, \boldsymbol{\alpha})$ is defined as,

$$g(R, \boldsymbol{\alpha})^{-1} = g(R^{-1}, -R^{-1}\boldsymbol{\alpha}). \tag{5}$$

Where we can easily show that,

$$\begin{aligned}
g(R,\boldsymbol{\alpha})^{-1}g(R,\boldsymbol{\alpha})\boldsymbol{r} &= g(R^{-1},-R^{-1}\boldsymbol{\alpha})g(R,\boldsymbol{\alpha})\boldsymbol{r} \\
&= g(R^{-1},-R^{-1}\boldsymbol{\alpha})\{R\boldsymbol{r}+\boldsymbol{\alpha}\} \\
&= R^{-1}(R\boldsymbol{r}+\boldsymbol{\alpha}) - R^{-1}\boldsymbol{\alpha} \\
&= R^{-1}R\boldsymbol{r} + R^{-1}\boldsymbol{\alpha} - R^{-1}\boldsymbol{\alpha} \\
&= E\boldsymbol{r} + 0 \\
&= \boldsymbol{r},
\end{aligned} \tag{6}$$

as we would expect. Therefore $g(R,\boldsymbol{\alpha})^{-1}g(R,\boldsymbol{\alpha}) = g(E,0)$.

One can easily check that the set of all symmetric operations $g(R,\boldsymbol{\alpha})$ equipped with the multiplication rule defined in Eq. 4 defines a group, which we will denote as S and is called the space group. Also, the set of rotations in $g(R,\boldsymbol{\alpha})$ which preserve the crystal invariance defines a group G called the point group.

There are many classification schemes for grouping space groups and point groups into classes which have many uses in crystallography and solid state physics, the interested reader in this material is encouraged to take a look at [2]. However, the goal here is not to dive deep in an application of group theory in CMP but rather to get a taste of different ways in which group theory arises in CMP leading to Bloch's theorem. With this being said let's keep on trucking and move on to to the group theory for Bloch's theorem.

Bloch's Theorem

Bloch's theorem is an important theorem often taught in introductory solid state physics which states that anytime you have a periodic potential, such as a the potential produced by atoms in a crystal lattice, you will have electron eigenstates of the form,

$$\psi(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}u_{\boldsymbol{k}}(\boldsymbol{r}), \tag{7}$$

which obey,

$$\hat{P}_{\{E|\boldsymbol{\tau}\}}\psi(\boldsymbol{r}) = \psi(\boldsymbol{r}+\boldsymbol{\alpha}) = e^{i\boldsymbol{k}\cdot\boldsymbol{\alpha}}\psi(\boldsymbol{r}).$$

$\hat{P}_{\{E|\boldsymbol{\tau}\}}$ is the translation operator *, $\boldsymbol{k}$ is a reciprocal lattice vector and $u_{\boldsymbol{k}}(\boldsymbol{r}+\boldsymbol{\alpha}) = u_{\boldsymbol{k}}(\boldsymbol{r})$ is a function that has the same periodicity as the crystal lattice.

In order to see where this came from we have to first understand reciprocal space (also known as k-space).

Reciprocal lattice vectors

The set of wave vectors $\boldsymbol{K}_m$ which yield plane waves with the same periodicity as the Bravais lattice defines a reciprocal lattice (k-space). These reciprocal lattice vectors $\boldsymbol{K}_m$ follow the following relation,

$$e^{\boldsymbol{K}_m\cdot(\boldsymbol{r}+\boldsymbol{l}_n)} = e^{\boldsymbol{K}_m\cdot\boldsymbol{r}}, \ \forall\ \boldsymbol{r}, \boldsymbol{l}_n, \text{ and } \boldsymbol{K}_m, \tag{8}$$

where again $\boldsymbol{r}$ is a point on the crystal lattice, $\boldsymbol{l}_n$ is a lattice vector, and $\boldsymbol{K}_m$ is a reciprocal lattice vector satisfying,

$$e^{\boldsymbol{K}_m\cdot\boldsymbol{l}_n} = 1. \tag{9}$$

Where,

$$\boldsymbol{l}_n = \sum_{i=1}^{3} n_i\boldsymbol{a}_i, \quad \boldsymbol{K}_m = \sum_{j=1}^{3} m_i\boldsymbol{b}_j, \text{ and } \quad \boldsymbol{b}_j\cdot\boldsymbol{a}_i = 2\pi\delta_{ij}.$$

*Here I have began to use the notation of [1].

From this we can easily see that in general,

$$\boldsymbol{K}_m \cdot \boldsymbol{l}_n = 2\pi N, \quad N \in \mathbb{Z}.$$

We now focus our attention to the translation operator $\hat{P}_{\{E|\boldsymbol{\tau}\}}$ which is the operator of the elements of $\mathcal{T}$, the translation subgroup which is a subgroup of S. This space group operator operator leaves the periodic potential invariant,

$$\hat{P}_{\{R|\boldsymbol{\tau}\}} V(\boldsymbol{r}) = V(\boldsymbol{r})$$

which is what we would expect. This property gives rise to the following result when, $\hat{P}_{\{E|\boldsymbol{\tau}\}}$ acts on a wave function,

$$\hat{P}_{\{E|\boldsymbol{\tau}\}} \psi(\boldsymbol{r}) = \psi(\boldsymbol{r} + \boldsymbol{\tau}).$$

With all this being said we now go on to prove Bloch's theorem.

Given that the translation group $\mathcal{T}$ is Abelian, the elements of $\mathcal{T}$ commute and the irreducible representations are one-dimensional. We will use the periodic boundary condition in which,

$$\{E|\boldsymbol{\tau}_1 + NL_1\} = \{E|\boldsymbol{\tau}_1\},$$

where $N \in \mathbb{Z}$ and L_1 is the length of the crystal along the direction of $\boldsymbol{a}_1$. This gives rise to a one-dimensional matrix representation of the the translation operator $\boldsymbol{\tau}_i = n_i \boldsymbol{a}_i,\ i = \{1, 2, 3\}$,

$$D^{k_1}(n_1 a_1) = e^{ik_1 n_1 a_1} = e^{ik_1 \tau_1}$$

since,

$$\hat{P}_R \psi(\boldsymbol{r}) = D^k(R) \psi_k(\boldsymbol{r}), \tag{10}$$

where the R here denotes a symmetry element, $k_1 = 2\pi m_1 / L_1$ corresponding to the m-th irreducible representation of the translation operator, and $m_1 = 1, 2, \cdots, (L_1/a_1)$. So for each m_1 there is a unique k_1 such that each irreducible representation if labeled by either m_1 or k_1 as indicated above. If now extend this argument for the general translation operator $\boldsymbol{tau}$ then the matrix representation is,

$$D^{k_1}(n_1 a_1) D^{k_2}(n_2 a_2) D^{k_3}(n_3 a_3) = e^{ik_1 n_1 a_1} e^{ik_2 n_2 a_2} e^{ik_3 n_3 a_3} = e^{i\boldsymbol{k}\cdot\boldsymbol{\tau}}.$$

This allows us to extend our result from Eq. N to produce,

$$\hat{P}_{\{E|\boldsymbol{\tau}\}} \psi(\boldsymbol{r}) = \psi(\boldsymbol{r}) e^{i\boldsymbol{k}\cdot\boldsymbol{\tau}} = e^{i\boldsymbol{k}\cdot\boldsymbol{\tau}} \psi(\boldsymbol{r}) = \psi(\boldsymbol{r} + \boldsymbol{\tau}),$$

yielding Bloch's theorem.

Q.E.D

References:

[1] Dresselhaus, Mildred S., et al. Group Theory: Application to the Physics of Condensed Matter. Springer-Verlag, 2010.
[2] Ma, Zhong-Qi. Group Theory for Physicists. World Scientific, 2007.