

Bloch's theorem and Bravais lattices

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We study the eigenstates of Hamiltonians $H = p^2/2m + V(x)$, where the potential $V(x)$ has the symmetry of some periodic lattice of points, e.g., the positions of atoms or ions in a crystalline solid. In particular, we prove Bloch's theorem, which provides a powerful ansatz for the eigenstates of such a Hamiltonian, and is the basis for the band structure of solids. *En route* to Bloch's theorem we introduce the basic language for the description of lattices, including the notion of a *Bravais lattice*, and the corresponding *reciprocal lattice*.

I. OVERVIEW

Determining the energy eigenstates of a quantum system is one of the most important problems of physics. For a complex many-body system this problem is, in general, fantastically difficult. Nonetheless, in condensed matter physics a tremendous amount of progress on this problem has been made by assuming some *periodic structure* in the system under consideration. *Bloch's theorem* gives us a great deal of information about the form of the energy eigenstates in such a system. The purpose of this note is to explain Bloch's theorem, together with the relevant prerequisite notions from the theory of lattices. The discussion is based on material from Chapters 4 through 8 of Ashcroft and Mermin [1].

II. BRAVAIS LATTICES

Many interesting materials and devices have some periodic structure, and the language of lattices is extremely useful in describing such structure. For example, in a crystalline conducting solid, we may describe conduction as the hopping of electrons from one ion to another, with the ions placed periodically throughout the crystal. In this section we introduce the basic language of lattices, including the concept of a Bravais lattice and its associated reciprocal lattice.

Suppose $\vec{a}_1, \dots, \vec{a}_m$ are a set of linearly independent vectors in some real vector space. We assume for later notational convenience that the vector space also has dimension m ; this assumption can be lifted without significantly changing our results. We define the *Bravais lattice* with *primitive vectors* $\vec{a}_1, \dots, \vec{a}_m$ to be the set of points that can be written in the form

$$\sum_j n_j \vec{a}_j, \quad (1)$$

where the n_j are all integers. The primitive vectors are said to *generate* or *span* the lattice. A simple example of a Bravais lattice is a square lattice in two dimensions, which has primitive vectors $\vec{a}_1 = (1, 0)$ and $\vec{a}_2 = (0, 1)$. I'd give other examples at this point, but to be really useful such examples should be accompanied by figures, and in a L^AT_EX document I think that's likely more trouble than it's worth. The reader should construct their own examples; it's also worth looking at the discussion in Ashcroft and Mermin [1], which has many very interesting examples.

Real physical systems are finite in extent, so a Bravais lattice can never be an accurate description of such a system. But in many systems of physical interest it is possible to ignore surface effects, and approximate the description of the system by a Bravais lattice. (This is yet another example of the interesting phenomenon that it is often much easier to describe infinite systems than finite systems.) Furthermore, in many physically occurring crystals the geometry is not that of a Bravais lattice with a *single* atom or ion at each lattice point, but rather are better understood as a Bravais lattice whose points correspond to some more complex primitive structure consisting of *several* atoms or ions. Ashcroft and Mermin [1] describe many interesting examples.

Given a Bravais lattice defined by primitive vectors $\vec{a}_1, \dots, \vec{a}_m$ it is also possible to define a natural *reciprocal* or *dual* lattice. The reciprocal lattice is defined by specifying a set of primitive vectors $\vec{b}_1, \dots, \vec{b}_m$ that are chosen to satisfy

$$\vec{b}_j \cdot \vec{a}_k = 2\pi\delta_{jk}. \quad (2)$$

This definition raises many questions. Can we always find such a set of vectors \vec{b}_j ? Even if we can, why make such a definition for a lattice? What is the physical significance of the reciprocal lattice? We'll try to answer all of these questions, starting by giving a recipe for constructing primitive vectors satisfying Eq. (2).

Before giving that recipe, however, we note an elegant definition of the reciprocal lattice that is equivalent to Eq. (2), and which will be useful later. Namely, the reciprocal lattice consists of those vectors \vec{k} satisfying

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$\exp(i\vec{k} \cdot \vec{r}) = 1$ for all \vec{r} in the Bravais lattice. The proof of equivalence is straightforward.

We'll give two approaches to the construction of the \vec{b}_j . The first approach is rather pedestrian, while the second is efficient. Depending on your predilections you may find either the first or the second a more transparent approach.

The pedestrian approach is as follows. To construct \vec{b}_1 , start by finding a vector \vec{v} that is orthogonal to $\vec{a}_2, \dots, \vec{a}_m$. This can be done, for example, by applying the Gram-Schmidt procedure to the vectors $\vec{a}_2, \dots, \vec{a}_m, \vec{a}_1$, in that order. The last vector produced by the Gram-Schmidt procedure is guaranteed to be orthogonal to all the vectors produced earlier by the Gram-Schmidt procedure, which span the same space as $\vec{a}_2, \dots, \vec{a}_m$. The vector \vec{b}_1 is now chosen by renormalizing \vec{v} so that $\vec{b}_1 \cdot \vec{a}_1 = 2\pi$. The vectors $\vec{b}_2, \dots, \vec{b}_m$ may be constructed similarly.

The efficient technique for finding $\vec{b}_1, \dots, \vec{b}_m$ satisfying Eq. (2) is to define an $m \times m$ matrix A whose columns are the vectors $\vec{a}_1, \dots, \vec{a}_m$. This is a square matrix, and the linear independence of $\vec{a}_1, \dots, \vec{a}_m$ ensures that it is invertible¹. Suppose we define an $m \times m$ matrix B whose columns are possible solutions to Eq. (2). A little thought shows that the condition Eq. (2) is equivalent to

$$B^T A = 2\pi I, \quad (3)$$

where I is the $m \times m$ identity matrix. The solution to this equation is $B = 2\pi(A^{-1})^T$, which gives an extremely simple and computationally efficient way of finding the primitive vectors for the reciprocal lattice.

A nice feature of this method is that it gives rise to a *unique* solution B , and thus shows that there is a unique set of primitive lattice vectors $\vec{b}_1, \dots, \vec{b}_m$ satisfying Eq. (2). This method can also be used to verify that the reciprocal of the reciprocal of a lattice is just the original lattice, since²

$$2\pi \left[(2\pi(A^{-1})^T)^{-1} \right]^T = A \quad (4)$$

Another way of seeing that the reciprocal of the reciprocal lattice is the original lattice is directly from Eq. (2), which makes it manifestly obvious that $\vec{a}_1, \dots, \vec{a}_m$ defines a lattice reciprocal to the lattice with primitive vectors $\vec{b}_1, \dots, \vec{b}_m$.

Having seen how to compute the reciprocal lattice, let us return to the question of the physical significance of

the reciprocal lattice. We've chosen to define the reciprocal lattice without giving any specific physical motivation. We'll see in the next section that the reciprocal lattice vectors arise naturally in the proof of Bloch's theorem, and there are many other places where the reciprocal lattice arises.

As an example, when doing X-ray diffraction experiments on crystals, a result due to Laue tells us that the peaks in intensity of the reflected X-rays occur when the change in momentum $\Delta\vec{k}$ of the X-ray radiation is an element of the reciprocal lattice. This condition lets us use X-ray diffraction experiments to determine the structure of the reciprocal lattice, and then take the reciprocal of the reciprocal lattice to determine the structure of the underlying lattice, and thus of the crystal! Of course, this only works if the underlying structure is that of a Bravais lattice; nonetheless, this procedure is astoundingly simple and elegant when one considers what is being determined — the structure of matter at the nanoscale³. I have been told that modern X-ray diffraction experiments (which are presumably variants on this basic idea) work so well that our best value for Avogadro's constant comes from such experiments.

While such examples are interesting, they do not answer the question of what the physical significance of the reciprocal lattice is. The question is really best answered by considering the general role played by abstraction in physics. There are many physical concepts which started life as mathematical definitions — consider examples such as the energy, the density matrix, the Lagrangian, even the notion of a force, or a field. A good physical understanding and interpretation of these concepts is developed when one connects them to many different physical phenomena, and builds up “intuition” — really, just rules of thumb about how those concepts affect other physical phenomena.

Of course, I'm begging the question: I'm not explaining the physical significance of the reciprocal lattice. What I am explaining is why we shouldn't necessarily expect it to make immediate physical sense. It's only when an abstract concept like the reciprocal lattice has been closely connected to several other physical phenomena that its physical content will make sense. We're not going to do that in this note, since the reciprocal lattice is peripheral to the main point of the note, which is to understand Bloch's theorem. In the absence of such connections, I believe that the best attitude to take to the reciprocal lattice is to transfer to physics von Neumann's dictum “Young man, in mathematics you don't understand things, you just get used to them.”

¹ We insisted earlier that a lattice with m primitive vectors live in an m -dimensional real vector space, not some higher-dimensional vector space. The reason for doing this was to make A an invertible square matrix. It's easy to modify the present construction when A is not an invertible square matrix, but it makes things a little more notationally complex, and thus less transparent.

² To prove this it helps to recall from basic linear algebra that $(X^T)^{-1} = (X^{-1})^T$.

³ I must admit, I don't know how to measure the wavelength of X-ray radiation. At optical frequencies there are straightforward interference experiments you can do to measure optical wavelengths (which is also a pretty amazing thing to be able to do); perhaps similar techniques also work well for the much shorter wavelength X-ray radiation.

III. BLOCH'S THEOREM

Suppose we are describing a quantum mechanical system with the symmetry of a Bravais lattice. For example, we might be describing the hopping of an electron from ion to ion in a crystalline conductor. In such a situation we expect that the Hamiltonian describing the system reflects the symmetry of the lattice, e.g.,

$$H = \frac{\vec{p}^2}{2m} + V(\vec{x}), \quad (5)$$

where the potential $V(\vec{x})$ satisfies $V(\vec{x}) = V(\vec{x} + \vec{r})$ for all \vec{r} in the lattice. Bloch's theorem tells us that in such a situation it is possible to choose a set of eigenstates for the Hamiltonian which are products of plane waves (i.e., momentum eigenstates) with functions having the periodicity of the lattice.

Theorem 1 (Bloch's theorem). *Let $H = \vec{p}^2/2m + V(\vec{x})$ be a single-particle Hamiltonian such that $V(\vec{x}) = V(\vec{x} + \vec{r})$ for all \vec{r} in some Bravais lattice. Then we can choose a set of eigenstates $|\psi\rangle$ for H such that in the position representation each eigenstate satisfies*

$$\psi(\vec{x}) = e^{i\vec{k}\cdot\vec{x}}\phi(\vec{x}), \quad (6)$$

for some vector \vec{k} , and for some function $\phi(\vec{x})$ satisfying $\phi(\vec{x} + \vec{r}) = \phi(\vec{x})$ for all \vec{r} in the lattice.

Bloch's theorem greatly simplifies the analysis of such Hamiltonians, giving us a general-purpose ansatz that we can use to solve the system. As a very simple example of Bloch's theorem in action, note that when $V(\vec{x}) = V_0$, a constant, Bloch's theorem tells us that we can choose the eigenstates of the Hamiltonian to be plane waves, i.e., momentum eigenstates. Thus, Bloch's theorem can be viewed as a generalization of the familiar fact that the eigenstates of a free particle are plane waves.

Proof: Suppose the Bravais lattice has primitive vectors $\vec{a}_1, \dots, \vec{a}_m$. Define corresponding displacement operators $D_j \equiv \exp(-i\vec{a}_j \cdot \vec{p})$. The effect of D_j is to displace the entire system by \vec{a}_j . Note that D_j is a unitary operator, and thus has eigenvalues of the form $e^{i\theta}$. It is straightforward to see that the D_j all commute with one another, and also with the Hamiltonian H . As a result, we can find an energy eigenbasis labelled by eigenvalues of the D_j operators, i.e., containing states $|\psi\rangle$ satisfying

$$D_j|\psi\rangle = e^{i\theta_j}|\psi\rangle, \quad (7)$$

for some set of phase factors θ_j . This tells us that if we displace the state $|\psi\rangle$, then the only effect is to pick up a phase θ_j . To connect this statement to Eq. (6) we choose $\vec{k} \equiv -\frac{1}{2\pi} \sum_j \theta_j \vec{b}_j$, where the \vec{b}_j are primitive vectors for the reciprocal lattice satisfying Eq. (2). Making this choice ensures that

$$\vec{k} \cdot \vec{a}_j = -\theta_j \quad (8)$$

Furthermore, we define $|\phi\rangle$ in the position representation by

$$\phi(\vec{x}) \equiv \exp(-i\vec{k} \cdot \vec{x})\psi(\vec{x}). \quad (9)$$

With this definition it is clear that Eq. (6) is satisfied, provided we can show that $\phi(\vec{x} + \vec{r}) = \phi(\vec{x})$ for all \vec{r} in the lattice. Making use of Eqs. (7)- (9) we see that:

$$\phi(\vec{x}) = \exp(-i\vec{k} \cdot \vec{x})\psi(\vec{x}) \quad (10)$$

$$= \exp(-i\vec{k} \cdot \vec{x})\langle \vec{x} + \vec{a}_j | D_j | \psi \rangle \quad (11)$$

$$= \exp(-i\vec{k} \cdot \vec{x}) \exp(i\theta_j) \psi(\vec{x} + \vec{a}_j) \quad (12)$$

$$= \exp(i\vec{k} \cdot \vec{a}_j) \exp(i\theta_j) \phi(\vec{x} + \vec{a}_j) \quad (13)$$

$$= \phi(\vec{x} + \vec{a}_j), \quad (14)$$

from which it follows that $\phi(\vec{x} + \vec{r}) = \phi(\vec{x})$ for all \vec{r} in the lattice.

QED

The vector \vec{k} provided by Bloch's theorem is known as the *crystal momentum*. It should not be confused with the ordinary physical momentum. Indeed, it is clear (and can easily be verified by a direct calculation) that states of the form of Eq. (6) will not, in general, be eigenstates of the usual momentum operator. Instead, the crystal momentum \vec{k} should be viewed simply as a quantum number that can be used to label the eigenstates of a Hamiltonian respecting the lattice symmetry.

In our statement of Bloch's theorem we have not said anything about the values of \vec{k} that are allowed. We will see that the values of \vec{k} can be restricted to lie in a region known as the *first Brillouin zone*. The first Brillouin zone is defined to be the set of \vec{k} vectors which are closer to (or as close too) the origin than they are to any other point in the reciprocal lattice. Observe that any point \vec{k} in \vec{k} -space can be written in the form

$$\vec{k} = \vec{k}_B + \vec{K}, \quad (15)$$

where \vec{k}_B is in the first Brillouin zone, and \vec{K} is the point in the reciprocal lattice closest to \vec{k} . It follows that

$$\exp(i\vec{k} \cdot \vec{x}) = \exp(i\vec{k}_B \cdot \vec{x}) \exp(i\vec{K} \cdot \vec{x}). \quad (16)$$

But $\exp(i\vec{K} \cdot \vec{r}) = 1$ whenever \vec{r} is in the Bravais lattice. This observation allows us to rewrite the wavefunction $\psi(\vec{x}) = \exp(i\vec{k} \cdot \vec{x})\phi(\vec{x})$ appearing in Bloch's theorem as $\psi(\vec{x}) = \exp(i\vec{k}_B \cdot \vec{x})\phi'(\vec{x})$, where $\phi'(\vec{x}) \equiv \exp(i\vec{K} \cdot \vec{x})\phi(\vec{x})$ satisfies $\phi'(\vec{x} + \vec{r}) = \phi'(\vec{x})$ for all \vec{r} in the Bravais lattice. It follows that without loss of generality we may suppose that the vectors \vec{k} appearing in Bloch's theorem may be restricted to vectors in the first Brillouin zone.

For any given value of \vec{k} there may be many different energy eigenstates. In general, we can label the energy eigenstates $|\psi_{\vec{k}n}\rangle$, where n is some other quantum number or set of quantum numbers. For a fixed value of \vec{k} , a

little algebra shows that the eigenvalue problem for $|\phi\rangle$ becomes

$$\left(\frac{(\vec{p} + \vec{k})^2}{2m} + V(x) \right) |\phi\rangle = E|\phi\rangle, \quad (17)$$

with boundary conditions $\phi(\vec{x} + \vec{r}) = \phi(\vec{x})$ for all \vec{r} in the Bravais lattice. It ought to seem plausible that the boundary conditions ensure a *discrete* (though possibly infinite) spectrum of energy eigenvalues, much as for a single particle in a potential well of infinite depth. In actual calculations, it is found that the energy eigenvalues $E_{\vec{k}_n}$ fall into separate *bands*, one band for each value of n , with the levels within a given band labelled by the different values of \vec{k} . The resulting energy level structure $E_{\vec{k}_n}$ is known as the *band structure* for the lattice. Calculations of this band structure play an extremely important role in the modern theory of conduction in metals.

IV. SUMMARY

Summary of material covered: definition of Bravais lattice; definition of the reciprocal lattice; how to find the reciprocal lattice; Bloch's theorem; crystal momentum; restriction of crystal momentum to the first Brillouin zone; concept of band structure.

Summary of main ideas: when trying to find the eigenstates of an operator with a periodic structure, start with Bloch's ansatz for the energy eigenstates.

Acknowledgments

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[1] N. W. Ashcroft and N. D. Mermin, *Solid state physics* (Harcourt Brace College Publishers, Fort Worth, 1976).