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Bloch's Theorem: A basis for the wavefunctions of electrons in crystalline solids

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ABSTRACT

Bloch functions serve as a suitable basis for the description of electrons in a periodic potential environment. In this paper, the translational symmetry of crystal lattice, their associated wave vectors in reciprocal lattice space and the simultaneous eigenfunctions of the Translation operator and Hamiltonian of the system have been taken into consideration to obtain the Bloch states of electrons.The Bloch's theorem is a cardinal result in the study of Solid state Physics, Condensed Matter Physics and Superconductivity of Materials.

1. Introduction

The Bloch theorem in essence formulates a condition that all solutions $\psi(\mathbf{r})$, for any periodic potential $V(\mathbf{r})$ whatsoever (in our case we are considering the wavefunctions of electrons being confined inside a perfectly crystalline solid), have to meet. This model attempts to derive the theorem by considering the quantum mechanical problem of a particle in a one-dimensional lattice to describe its behaviour in a periodic crystal lattice. Assuming the hypothesis of a fixed infinite periodic potential, A Bloch wave function can be described in the form of a plane-wave modulated by a periodic function (with the periodicity of the crystal). Furthermore, this result has a remarkable impact in describing the Meissner effect (in the microscopic theory of superconductivity) using the canonical momentum arguments and taking the classical description of Current Density to a quantum mechanical one; to justify the London equations. (London & London (1935))

2. Theory

The defining property of a crystal is translational symmetry, so upon moderating the state of a wavefunction of electron in position space (or in the momentum space) slightly, all the properties of the wavefunction stays invariant and the electron would have no idea about the relocation. We can utilize this characteristic behaviour to prove the functional form of Bloch's theorem as follows;

A three-dimensional crystal has three primitive lattice vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$. If the crystal is shifted by any of these three vectors, or a combination of them of the form (Ashcroft et al. (1976))

$$n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 \tag{1}$$

Where, n_i are integers; then the atoms end up in the same set of locations as they started, and it becomes impossible to differentiate the translational movement happening within the crystal.

It is also convenient to introduce the concept of the reciprocal lattice vectors. In solid-state physics, the reciprocal lattice is basically the Fourier transform of the direct lattice, which is usually a periodic function in time. While the direct lattice (e.g., a lattice of a crystal) exists in real space, the reciprocal lattice exists in reciprocal space (also known as momentum space or K-space).(Dresselhaus et al. (2008))

Here, these are three vectors b_1, b_2, b_3. Now, we define the translation operator (in Dirac notation)

$$\hat{\mathbf{T}}_\mathbf{n}\psi(\mathbf{r}) = \psi(\mathbf{r}+\mathbf{T}_\mathbf{n}) = \psi(\mathbf{r}+n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3) = \psi(\mathbf{r}+\mathbf{n}\cdot\mathbf{a}) \tag{2}$$

We use the hypothesis of a mean periodic potential

$$U(\mathbf{x}+\mathbf{T}_\mathbf{n}) = U(\mathbf{x}) \tag{3}$$

We can also write the Hamiltonian of the system

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + U(\mathbf{x}) \tag{4}$$

Given that it is invariant for translations, the lattice symmetry translation operator shall commute with the system's Hamiltonian.

$$[\hat{H}, \hat{\mathbf{T}}_\mathbf{n}] = 0 \tag{5}$$

And the two operators will reflect a common set of eigenfunctions. Therefore we can look at the eigenfunctions of the operator

$$\hat{\mathbf{T}}_\mathbf{n}\psi(\mathbf{x}) = \lambda_\mathbf{n}\psi(\mathbf{x}) \tag{6}$$

Also, $\hat{\mathbf{T}}_\mathbf{n}$ is an additive operator, with the property

$$\hat{\mathbf{T}}_{\mathbf{n_1}}\hat{\mathbf{T}}_{\mathbf{n_2}}\psi(\mathbf{x}) = \psi(\mathbf{x}+\mathbf{n_1}\cdot\mathbf{a}+\mathbf{n_2}\cdot\mathbf{a}) = \hat{\mathbf{T}}_{\mathbf{n_1}+\mathbf{n_2}}\psi(\mathbf{x}) \tag{7}$$

So from the eigenvalue equation, we have

$$\lambda_{\mathbf{n}_1}\lambda_{\mathbf{n}_2} = \lambda_{\mathbf{n}_1+\mathbf{n}_2} \tag{8}$$

This is true for

$$\lambda_\mathbf{n} = e^{s\mathbf{n}\cdot\mathbf{a}} \tag{9}$$

Where s is a complex number. (i.e., $s \in C$) So from the Normalization of wavefunctions, we get $|\lambda_\mathbf{n}|^2 = 1$ And $s = ik$. Here we have defined $k = m_1b_1 + m_2b_2 + m_3b_3$, and b_j are the reciprocal lattice vectors.

So we finally get,

$$\hat{\mathbf{T}}_\mathbf{n}\psi(\mathbf{x}) = \psi(\mathbf{x}+\mathbf{n}\cdot\mathbf{a}) = e^{ik\mathbf{n}\cdot\mathbf{a}}\psi(\mathbf{x}) \tag{10}$$

And, if a wave function is an eigenstate of all of the translation operators (simultaneously), then it is a Bloch state. So, for a Bloch wave,

$$\psi_\mathbf{k}(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}u_\mathbf{k}(\mathbf{x}) \tag{11}$$

with $u_\mathbf{k}(\mathbf{x}) = u_\mathbf{k}(\mathbf{x}+\mathbf{n}\cdot\mathbf{a})$. where u is periodic, with the same periodicity as the atomic structure of the crystal.

3. Results

This theorem asserts that solutions to the Schrödinger equation in a periodic potential take the form of a plane wave function adjusted by a periodic function. They are written mathematically as Equation 11.

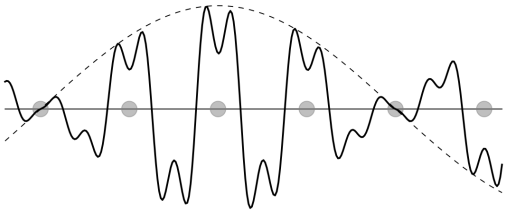

Fig. 1. Solid line: A schematic of the real part of a typical Bloch wave in one dimension. The dotted line is from the $e^{ik \cdot x}$ factor (being in the complex plane). And the light circles represent atoms in the crystal lattice.

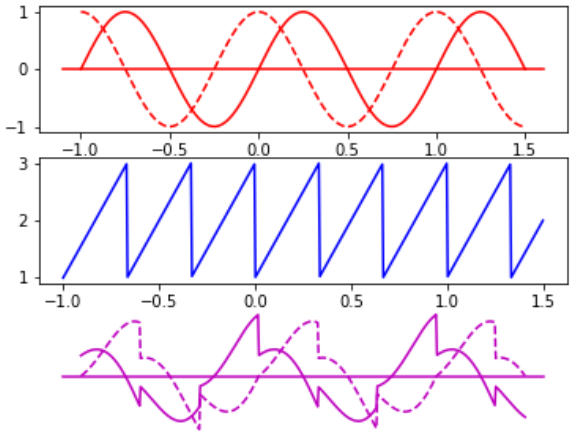

Fig. 2. The figure on top, stands for the complex roots of unity $e^{ik \cdot x}$ where the solid red line is the real part and the dotted line is the imaginary part of it. the graph shown in the middle is the representation of Saw-tooth function (an arbitrary periodic function) to be multiplied with the complex unity factor to result in the following (bottom) wavefunction of electrons (again, where the solid magenta line is the real part and the dotted line is the imaginary part)

As mentioned in the above figures 1, The wave vector k has a special significance as "the quantum number of translation" and provides a label for the irreducible representations of the translation group.(Kittel et al. (1996))

In the figure 2, $f(x) = 2 + scipy.signal.sawtooth(6 * numpy.pi * x)$ is the periodic function used, to be multiplied with the complex exponential factor and the wavefunction of electron in the crystal can be visualized as in the plot (in magenta).

4. Discussion

In addition to the applicability of the Bloch's Theorem in characterizing the electronic properties of crystals (especially the electronic band structure); its pertinence extends more fundamentally to any wave-like phenomenon in a periodic medium. The actual quantum state of an electron in crystalline solid can entirely be described by the wavefunction ψ and as described in the Equation 11, it is written using the reciprocal lattice vector $\mathbf{k}$ which is only unique to each Bloch state within a restricted set of values, namely The first Brillouin zone (in k-space).(Landau & Lifshitz (1977)) Interestingly, when k is multiplied by the reduced Planck's constant, it equals the electron's crystal momentum (or quasi-momentum). Related to this, the group velocity of an electron can be calculated based on how the energy of a Bloch state varies with k. (Landau & Lifshitz (1977))

5. Conclusions

By relating the translational symmetry of a crystal in its primitive lattice and reciprocal lattice vectors, we were able to construct an instrumental method to obtain the Bloch's Theorem for electrons in a perfect crystal. Based on the invariant nature of the crystal along the its translational axis, we concluded that the translational operator $\hat{\mathbf{T}}_\mathbf{n}$ and the Hamiltonian of the system $\hat{H}$ commutes with each other and consequently the two operators will have a common set of eigenfunctions. This, in turn, explicitly yields that the wavefunction is an eigenstate of all of the translation operators simultaneously; and it serves as a suitable basis for the wavefunctions of electrons in crystalline solids. This method of deriving the Bloch's Theorem using operators, provides significant insight in modelling electrons as quantum mechanical particles travelling through a fixed infinite periodic potential.

References

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