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AN ANALOGUE OF THE BLOCH THEOREM IN FOUR DIMENSIONS

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Synopsis

An analogue of the Bloch theorem is proved for the case of an electron in the presence of a crystal potential and a monochromatic radiation field.

Recently Nickle[1]) has shown that the problem of solving the Schrödinger equation of an electron in the presence of a simple cubic crystal potential and monochromatic laser radiation can be simplified by making use of certain symmetry properties of the corresponding time-dependent Hamiltonian. Essentially two "Ansätze" were used (see eqs. (8) and (20) of I) which provided information on the general form of the solutions of the Schrödinger equation. Nickle suggested that "if the Hamiltonian were not explicitly time dependent" eq. (20) of I could be proved.

In this note we wish to show that there exists an analogue of the Bloch theorem for an electron in the presence of a periodic potential (without restricting the lattice to be simple cubic), and a monochromatic radiation field. To prove this theorem we shall make use of the fact that the Schrödinger equation and the corresponding Hamiltonian are invariant under a certain space–time group which contains as a proper subgroup the symmetry transformations considered in I. In the special case of a simple cubic lattice this theorem reduces to the Ansatz of I apart from separation of variables which does not follow from symmetry arguments.

Let $V(\boldsymbol{r})$ be an arbitrary periodic crystal potential and $\boldsymbol{A}(\boldsymbol{r}, t)$ be the vector potential corresponding to a given monochromatic radiation field. The Schrödinger equation of an electron in the presence of the potentials $\boldsymbol{A}(\boldsymbol{r}, t)$ and $V(\boldsymbol{r})$ is

$$\mathrm{i}\,\frac{\partial}{\partial t}\,\psi(\boldsymbol{r}, t) = H(\boldsymbol{r}, \boldsymbol{p}, t)\,\psi(\boldsymbol{r}, t); \tag{1}$$

$$H(\boldsymbol{r}, \boldsymbol{p}, t) = \frac{1}{2m}\,(\boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{r}, t))^2 + eV(\boldsymbol{r}) \qquad (c = \hbar = 1), \tag{2}$$

where $A(\boldsymbol{r}, t) = \boldsymbol{A}\, e^{i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)}$. (Here we use Coulomb's gauge, div $A(\boldsymbol{r}, t) = 0$; $\boldsymbol{k}$ and ω are the wave vector and angular frequency of the radiation field, respectively.) Let $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, $\boldsymbol{a}_3$ be three linearly independent primitive lattice vectors, and $\boldsymbol{a}_1^*$, $\boldsymbol{a}_2^*$, $\boldsymbol{a}_3^*$ the corresponding reciprocal lattice vectors. Let $k = (\boldsymbol{k}, \omega)$ be the four-vector of the radiation field and denote by Λ_k^* the four dimensional space–time lattice generated by the vectors $(\boldsymbol{a}_1^*, 0)$, $(\boldsymbol{a}_2^*, 0)$, $(\boldsymbol{a}_3^*, 0)$ and k. It can be shown [2]) that the basis vectors of the four-dimensional space–time lattice dual to Λ_k^* are

$$b_1 = (\boldsymbol{a}_1, k_1\lambda),\ b_2 = (\boldsymbol{a}_2, k_2\lambda),\ b_3 = (\boldsymbol{a}_3, k_3\lambda),\ b_4 = (0, -\lambda)^{\ddagger}$$

where k_1, k_2, k_3 are given by $\boldsymbol{k} = k_1\boldsymbol{a}_1^* + k_2\boldsymbol{a}_2^* + k_3\boldsymbol{a}_3^*$ and $\lambda = 2\pi/\omega$. From eq. (2) it is easy to verify that the Hamiltonian $H(\boldsymbol{r}, \boldsymbol{p}, t)$ and hence the Schrödinger equation are invariant under the translation

$$x = (\boldsymbol{r}, t) \to x + n, \qquad n = n_1b_1 + n_2b_2 + n_3b_3 + n_4b_4 \tag{3}$$

(n_1, n_2, n_3, n_4 are integers). It follows that the operator

$$\begin{aligned} T_k(n) &= \exp\left\{n_1\frac{\partial}{\partial\xi_1} + n_2\frac{\partial}{\partial\xi_2} + n_3\frac{\partial}{\partial\xi_3} + n_4\frac{\partial}{\partial\xi_4}\right\} = \\ &= \prod_{i=1}^{3} \exp\left\{n_i(\boldsymbol{a}_i, k_i\lambda)\cdot\left(\boldsymbol{\nabla}, -\frac{\partial}{\partial t}\right)\right\} \exp\left\{-n_4\lambda\frac{\partial}{\partial t}\right\} \end{aligned} \tag{4}$$

commutes with $H(\boldsymbol{r}, \boldsymbol{p}, t)$. In eq. (4) the variables ξ_1, ξ_2, ξ_3 and ξ_4 are defined by the equation

$$x = x_1e_1 + x_2e_2 + x_3e_3 + x_4e_4 = \xi_1b_1 + \xi_2b_2 + \xi_3b_3 + \xi_4b_4$$

and

$$(\boldsymbol{\nabla}, 0) = e_1\frac{\partial}{\partial x_1} + e_2\frac{\partial}{\partial x_2} + e_3\frac{\partial}{\partial x_3}.$$

It is easy to check that $\xi_i = \beta_{ij}x_j$, $\xi_4 = \beta_{ji}x_ik_j - (t/\lambda)$ $(i, j = 1, 2, 3;\ \beta_{ij} = (\boldsymbol{a}_i, 0)\cdot e_j)$. The effect of $T_k(n)$ operating on any function $f(x)$ is

$$\begin{aligned} T_k(n)\, f(x) &= f(x + n) = \\ &= f(x + (n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3,\ k_1n_1\lambda + k_2n_2\lambda + k_3n_3\lambda - n_4\lambda)). \end{aligned} \tag{5}$$

If we change variables from x_1, x_2, x_3, t to ξ_1, ξ_2, ξ_3, ξ_4 such that

$$f(x) = f(x_1, x_2, x_3, t) = F(\xi_1, \xi_2, \xi_3, \xi_4),$$

then eq. (5) can also be written as

$$T_k(n)\, F(\xi_1, \xi_2, \xi_3, \xi_4) = F(\xi_1 + n_1, \xi_2 + n_2, \xi_3 + n_3, \xi_4 + n_4). \tag{6}$$

‡ See ref. 2 for the notations and the definitions of the basis four-vectors e_1, e_2, e_3, e_4, and the corresponding metric tensor.

The set of operators $T_k(n)$ for all integral values of n_1, n_2, n_3 and n_4 forms an Abelian group under the usual operator multiplication and will be denoted by $\tilde{T}_k$. The group of symmetry transformations considered in I is isomorphic to a subgroup of $\tilde{T}_k$ in which the parameter n_3 is set equal to n_4 (for the case of a simple cubic crystal and $\boldsymbol{k}$ parallel to $\boldsymbol{a}_3$).

It is clear that the group $\tilde{T}_k$ can be regarded as a direct product of four Abelian groups characterized by the integral parameters n_1, n_2, n_3 and n_4, respectively:

$$\tilde{T}_k = \tilde{T}_k^{(1)} \otimes \tilde{T}_k^{(2)} \otimes \tilde{T}_k^{(3)} \otimes \tilde{T}_k^{(4)}. \tag{7}$$

The general element of the group $\tilde{T}_k^{(\mu)} (\mu = 1, 2, 3, 4)$ is $\exp(n_\mu\, \partial/\partial\xi_\mu)$. Hence all the irreducible representations of $\tilde{T}_k$ must be one-dimensional and are given by

$$\Gamma^{(\kappa)}\{T_k(n)\} = \mathrm{e}^{2\pi\mathrm{i}(\kappa_1 n_1 + \kappa_2 n_2 + \kappa_3 n_3 - \kappa_4 n_4)} = \mathrm{e}^{\mathrm{i}\kappa\cdot n}, \tag{8}$$

where $\kappa = (\kappa_1 \boldsymbol{a}_1^* + \kappa_2 \boldsymbol{a}_2^* + \kappa_3 \boldsymbol{a}_3^* + \kappa_4 \boldsymbol{k},\ \kappa_4 \omega)$ and κ_1, κ_2, κ_3, κ_4 are real numbers such that $0 \leq \kappa_1, \kappa_2, \kappa_3, \kappa_4 < 1$.

By the method of projection operators[3] we can obtain a generating function $\psi_\kappa(x)$ of the irreducible representation $\Gamma^{(\kappa)}(\tilde{T}_k)$ from an arbitrary function $\phi(x)$:

$$\begin{aligned} \psi(x) &= \sum_{n_1} \sum_{n_2} \sum_{n_3} \sum_{n_4} (\Gamma^{(\kappa)}\{T_k(n)\})^* \, T_k(n)\, \phi(x) = \\ &= \mathrm{e}^{\mathrm{i}\kappa\cdot x} \Big[\sum_{n_1} \sum_{n_2} \sum_{n_3} \sum_{n_4} \mathrm{e}^{-\mathrm{i}\kappa(x+n)} \phi(x + n)\Big]. \end{aligned} \tag{9}$$

The expression inside the square brackets‡ of eq. (9) is invariant under the group $\tilde{T}_k$. Hence the solutions of the Schrödinger equation can be written in the form $\mathrm{e}^{\mathrm{i}\kappa\cdot x}\, u_\kappa(x)$ where $u_\kappa(x)$ is invariant under the group $\tilde{T}_k$, and this is the analogue of the Bloch theorem we want to prove.

In the special case of a simple cubic crystal with the coordinate axes chosen along the mutually perpendicular primitive lattice vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, $\boldsymbol{a}_3$

$$\left(i.e.\ e_1 = \left(\frac{\boldsymbol{a}_1}{a}, 0\right), e_2 = \left(\frac{\boldsymbol{a}_2}{a}, 0\right),\ e_3 = \left(\frac{\boldsymbol{a}_3}{a}, 0\right); \right.$$

$$\left. |\boldsymbol{a}_1| = |\boldsymbol{a}_2| = |\boldsymbol{a}_3| = a\right),$$

and the wave vector $(\boldsymbol{k}, 0)$ parallel to e_3

$$\left(i.e.\ (\boldsymbol{k}, 0) = \frac{2\pi}{\lambda} e_3\right)$$

‡ In eq. (9) we assume that the sums over all the elements of the group $\tilde{T}_k$ exist. To avoid the difficulty of dealing with infinite sums arising from the fact that $\tilde{T}_k$ is infinite we could introduce the periodic boundary conditions.

the solutions of the Schrödinger equation can be written in the form:

$$\psi(x) = \mathrm{e}^{\mathrm{i}\kappa\cdot x}\, u_\kappa(x) = \mathrm{e}^{(2\pi\mathrm{i}/a)(\kappa_1 x_1 + \kappa_2 x_2)}\, \mathrm{e}^{(2\pi\mathrm{i}/\lambda)(x_3 - t)}\, F_\kappa(x), \tag{10}$$

where

$$F_\kappa(x) = \mathrm{e}^{(2\pi\mathrm{i}/a)(\kappa_3 x_3)}\, u_\kappa(x). \tag{11}$$

In I, the solutions of the Schrödinger equation are assumed to be in the form

$$\mathrm{e}^{(2\pi\mathrm{i}/a)(\kappa_1 x_1 + \kappa_2 x_2)}\, \mathrm{e}^{(2\pi\mathrm{i}/\lambda)(x_3 - t)} \cdot G_\kappa(x)$$

as we have just proved. In addition, it is assumed that separation of variables in $G_\kappa(x)$ is possible. However, apart from the fact that we can write $G_\kappa(x)$ as a product of two functions as in eq. (11), the possibility of separating the variables does not follow from the symmetry argument.

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2) Janner, A. and Ascher, E., Physica **45** (1969) 33.
3) See, for example, Wigner, E., Group theory and its application to the quantum mechanics of atomic spectra, Academic Press (New York, 1959).