722 (1966), and 153, 802 (1967).

[3]W. Martienssen, J. Phys. Chem. Solids 2, 257 (1957), and 8, 294 (1959).

[4]D. Dutton, Phys. Rev. 112, 785 (1958).

[5]J. Hartke and P. Regensburger, Phys. Rev. 139, A970 (1965); K. J. Siemsen and E. W. Fenton, Phys. Rev. 161, 632 (1967). See also Halperin and Lax, Ref. 2.

[6]I. Nakada, J. Phys. Soc. Japan 20, 346 (1965); A. Matsui, J. Phys. Soc. Japan 21, 2212 (1966).

[7]For reviews, see C. C. Klick and J. H. Schulman, Solid State Physics, edited by F. Seitz and D. Turnbull (Academic Press, Inc., N. Y., 1957), and D. L. Dexter, ibid. (1958), Vol. 6.

[8]Toyozawa, Ref. 2.

[9]I am indebted to G. Gaspari, I. J. Kim, and W.-M. Shyu for their programs and assistance in the numerical integration of Eq. (5). Keil (Ref. 2) has noted the relationship between S and a Bessel function of the second kind, of imaginary argument.

[10]K. Kobayashi and T. Tomiki, J. Phys. Chem. Solids 22, 73 (1961).

[11]H. Mahr, Phys. Rev. 125, 1510 (1962).

[12]C. Klick, D. Patterson, and R. Knox, Phys. Rev. 133, A1717 (1964).

[13]M. Stevens and M. Menes, private communication of preliminary results, to be published.

[14]D. Redfield, Bull. Am. Phys. Soc. 9, 288 (1964).

FINITE TRANSLATIONS IN SOLID-STATE PHYSICS

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Eigenvalues of finite translations are used for specifying a complete set of states in quantum mechanics. A derivation of these states is given and they are shown to be very useful in solid-state physics.

It is shown that finite translations in direct and reciprocal space can be chosen to form a complete set of commuting operators in quantum mechanics.[1] The eigenfunctions of these operators are found and are proven to form a complete orthonormal set of functions. Expressions for the basic operators $\vec{r}$ and $\vec{p}$ have been derived in the representation of these functions.

The new complete set of functions are of the Bloch-type with the ideal feature of being expressible in infinitely localized Wannier functions. This makes them extremely useful in solid-state physics. As an example, the problem of an electron in a periodic potential and a constant magnetic field is considered. This problem has attracted attention for many years, and although the results expressed in the effective-mass approximation are very simple, their derivation is "shockingly complicated."[2] It was pointed out[3-5] that the complications come about because of the set of functions one uses for expanding the solution of the mentioned problem. It turns out that the functions obtained in this paper form a very convenient set for expanding the solutions of a Bloch electron in a magnetic field and give us a very good insight into the problem. This is demonstrated by deriving an equation that was used before[4,6,7] and shown to be very useful, but never rigorously proven.

Finite translations in real space,

$$T(\vec{R}_n) = \exp(i\vec{p}\cdot\vec{R}_n), \tag{1}$$

where $\vec{R}_n$ is a Bravais lattice vector and $\vec{p}$ is the linear-momentum operator ($\hbar = 1$), are known to be very important in solid-state physics. By means of them Bloch functions[8] $\psi_k(\vec{r})$ are defined:

$$T(\vec{R}_n)\psi_k(\vec{r}) = \psi_k(\vec{r}+\vec{R}_n) = \exp(i\vec{k}\cdot\vec{R}_n)\psi_k(\vec{r}). \tag{2}$$

Here $\vec{k}$ is the wave vector and it defines the eigenvalues of the translation operators $T(\vec{R}_n)$. Relation (2) does not define the Bloch functions completely; it only requires that they have the form[8]

$$\psi_k(\vec{r}) = \exp(i\vec{k}\cdot\vec{r})u_k(\vec{r}), \tag{3}$$

where $u_k(\vec{r})$ is an arbitrary periodic function, $u_k(\vec{r}+\vec{R}_n) = u_k(\vec{r})$. The reason that the operators $T(\vec{R}_n)$ do not define the functions ψ_k completely is because they do not form a complete set of commuting operators. It can be checked that operators

$$T(\vec{K}_m) = \exp(i\vec{r}\cdot\vec{K}_m) \tag{4}$$

with $\vec{K}_m$ being any vector of the reciprocal lattice commute with $T(\vec{R}_n)$, for any $\vec{R}_n$. This follows from the commutation relation between $\vec{p}$ and $\vec{r}$ and from the definition of the vectors $\vec{K}_m$ for the reciprocal lattice,[8] $\vec{K}_m \cdot \vec{R}_n = 2\pi l$ with integer l. Of course, the fact that $T(\vec{R}_n)$ and $T(\vec{K}_m)$ commute does not violate the uncertainty principle. The next statement is that operators which are functions of $\vec{r}$ and $\vec{p}$ and which commute with all the set $T(\vec{R}_n)$ and $T(\vec{K}_m)$ can depend only on $T(\vec{R}_n)$ and $T(\vec{K}_m)$. To prove this statement we use the theorem that any function of the operators $\vec{r}$ and $\vec{p}$, $f(\vec{r},\vec{p})$, can be Fourier analyzed by means of the operators[9] $\exp(i\vec{\alpha}\cdot\vec{p})$ and $\exp(i\vec{\beta}\cdot\vec{r})$ with $\vec{\alpha}$ and $\vec{\beta}$ running from $-\infty$ to ∞. Therefore, if $f(\vec{r},\vec{p})$ commutes with $T(\vec{R}_n)$ and $T(\vec{K}_n)$, it has to be a function of them only. This completes the proof that $T(\vec{R}_n)$ and $T(\vec{K}_m)$ for all possible $\vec{R}_n$ and $\vec{K}_m$ form a complete set of operators.

Having proven that the operators (1) and (4) form a complete set, we now find their eigenfunctions. Instead of deriving these functions,[10] we write them down and verify their correctness:

$$\psi_{kq}(\vec{r}) = \left[\frac{\tau}{(2\pi)^3}\right]^{1/2} \sum_{\vec{R}_n} \delta(\vec{q}-\vec{r}-\vec{R}_n)\exp(-i\vec{k}\cdot\vec{R}_n). \quad (5)$$

Here τ is the volume of a unit cell in the Bravais lattice and δ is the Dirac δ function.

It is easy to check that

$$T(\vec{R}_n)\psi_{kq}(\vec{r}) = \exp(i\vec{k}\cdot\vec{R}_n)\psi_{kq}(\vec{r}), \quad (6)$$

$$T(\vec{K}_m)\psi_{kq}(\vec{r}) = \exp(i\vec{q}\cdot\vec{K}_m)\psi_{kq}(\vec{r}). \quad (7)$$

Since the operators $T(\vec{R}_n)$ and $T(\vec{K}_m)$ form a complete set, Eqs. (6) and (7) define the functions ψ_{kq} up to an arbitrary phase factor (see below). The vectors $\vec{k}$ and $\vec{q}$ define the eigenvalues of the operators $T(\vec{R}_n)$ and $T(\vec{K}_m)$ correspondingly. $\vec{k}$ assumes values in the usual Brillouin zone, while $\vec{q}$ varies in a unit cell of the Bravais lattice (or a Brillouin zone in the direct lattice). The orthonormality of $\psi_{kq}(\vec{r})$ can be easily checked. One has

$$\int \psi_{k'q'}^*(\vec{r})\psi_{kq}(\vec{r})d^3r = \delta(\vec{k}'-\vec{k})\delta(\vec{q}'-\vec{q}). \quad (8)$$

It is interesting to compare the functions $\psi_{kq}(\vec{r})$ with the Bloch functions (3). Both of them are Bloch-type functions [relations (2) and (6)]. The former are specified by two continuous vectors $\vec{k}$ and $\vec{q}$, while the Bloch functions (3) depend on the $\vec{k}$ vector and a discrete band index n that comes from the energy operator.[8] In the functions $\psi_{kq}(\vec{r})$ the role of the discrete band index is taken by the continuous vector $\vec{q}$, a fact which is of great practical importance because it is usually much easier to work with differential equations than with equations in matrix form. This feature will become apparent in the example that is treated below.

Relation (5) can be looked at as an expansion of a Bloch-type function ψ_{kq} in infinitely localized Wannier functions.[4] This feature makes the functions ψ_{kq} extremely useful in describing the dynamics of Bloch electrons in external fields.[4]

As was already mentioned, Eqs. (6) and (7) do not fix the phase of $\psi_{kq}(\vec{r})$. The choice that was made in (5) turns out to be very convenient because the operators $\vec{r}$ and $\vec{p}$ have then the following simple form in the kq representation[10]:

$$\vec{r} = i\partial/\partial\vec{k} + \vec{q}, \quad (9)$$

$$\vec{p} = -i\,\partial/\partial\vec{q}. \quad (10)$$

This completes the construction of a new representation in quantum mechanics: a complete set of commuting operators (1) and (4), a complete set of functions (5), and the representation of the basic operators $\vec{r}$ and $\vec{p}$. Although during the construction we have explicitly used vectors $\vec{R}_n$ of a Bravais lattice and vectors $\vec{K}_m$ of a reciprocal lattice which are concepts in solid-state physics, the represtation is not necessarily related to solids because the two lattices mentioned can always be formally defined. There is, however, no doubt that this is a natural representation for problems in solids.

As an example let us derive an equation for a Bloch electron in a magnetic field. We start with the Schrödinger equation in the r representation for the symmetric gauge $\vec{A} = \frac{1}{2}[\vec{H}\times\vec{r}]$:

$$\{(2m)^{-1}[\vec{p} + (e/2c)\vec{H}\times\vec{r}]^2 + V(\vec{r})\}\psi(\vec{r}) = \epsilon\psi(\vec{r}), \quad (11)$$

where $\vec{H}$ is a constant magnetic field and $V(\vec{r})$ is the periodic potential. The function $\psi(\vec{r})$ can be expanded in the complete set of functions $\psi_{kq}(\vec{r})$:

$$\psi(\vec{r}) = \int C(\vec{k},\vec{q})\psi_{kq}(\vec{r})d^3k\,d^3q. \quad (12)$$

From the definition (5) of ψ_{kq} it follows that

$$C(\vec{k}+\vec{K}_m,\vec{q})=C(\vec{k},\vec{q}) \text{ and } C(\vec{k},\vec{q}+\vec{R}_n)=\exp(i\vec{k}\cdot\vec{R}_n)C(\vec{k},\vec{q}), \tag{13}$$

$$\left[(2m)^{-1}\left\{-i\frac{\partial}{\partial\vec{q}}+\frac{e}{2c}\left[\vec{H}\times\left(\vec{q}+i\frac{\partial}{\partial\vec{k}}\right)\right]\right\}^2+V(\vec{q})\right]C(\vec{k},\vec{q})=\epsilon C(\vec{k},\vec{q}), \tag{14}$$

where $C(\vec{k},\vec{q})$ are Bloch-type functions satisfying relations[11] (13). The difference between $C(\vec{k},\vec{q})$ and the ordinary Bloch functions (3) is that in the former, the vector $\vec{k}$ is no longer a constant of motion but appears as a variable in the equation.

In comparing Eq. (14) with the equation one obtains in the effective-mass approximation[2] (EMA) by expanding $\psi(\vec{r})$ in (12) not according to $\psi_{kq}(\vec{r})$ but in regular Bloch functions $\psi_{nk}(\vec{r})$, one finds that the band index which leads to a coupled set of equations in the EMA is replaced in (14) by a continuous variable. An equation of type (14) was first predicted by Wannier and Fredkin[4] from a heuristic argument and very interesting results were drawn from it. In more recent publications[6,7] Eq. (14) itself was constructed (up to a phase transformation) and shown to be useful for deriving the EMA in an extremely simple way. However, only now having an exact proof of Eq. (14), it becomes clear what is the meaning of the variables in this equation and what is the connection between $C(\vec{k},\vec{q})$ and the wave function in the r representation.

The example above shows that by use of the kq representation, the Bloch part of the Hamiltonian and the part that corresponds to the motion in the potential of the perturbation (the magnetic field in this example) appear in the equation side by side with a coupling between them. As is known,[8] this feature of having motions separated corresponds to the general behavior of electrons in perturbed crystals. It follows, therefore, that the representation constructed in this paper is of very great use in solid-state physics.

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[1]P. A. M. Dirac, The Principles of Quantum Mechanics (Oxford University Press, New York, 1947).

[2]W. Kohn, Phys. Rev. 115, 1460 (1959).

[3]Laura M. Roth, J. Phys. Chem. Solids, 23, 433 (1962).

[4]G. H. Wannier and D. R. Fredkin, Phys. Rev. 125, 1910 (1962).

[5]J. Zak, Phys. Rev. 136, A776 (1964).

[6]H. C. Praddaude, Phys. Rev. 140, A1292 (1965).

[7]P. G. Harper, J. Phys. Chem. Solids, 82, 495 (1967).

[8]C. Kittel, Quantum Theory of Solids (John Wiley & Sons, Inc., New York, 1963).

[9]H. J. Groenewold, Physica 12, 405 (1946).

[10]Their explicit derivation will be given elsewhere.

[11]In Ref. (7) it is claimed that $U(\vec{\chi},\vec{r})$ is periodic in both arguments. This is incorrect as can be seen from the same reference, where it is shown that for vanishing magnetic fields, U turns into the periodic part of the Bloch function which is known not to be periodic in $\vec{k}$.