Lattice operators in crystals for Bravais and reciprocal vectors*

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The kq representation is used for defining lattice operators whose eigenvalues are all the discrete vectors of the direct and the reciprocal lattices in crystals. The eigenstates of the lattice operators form a complete and orthonormal set of localized functions in both the configuration and the momentum spaces. It is shown that these eigenstates can be chosen to be closely connected to either the free electron or the extremely tightly bound electron Wannier functions. The lattice operators turn out to be conjugate to the k and q coordinates.

The concepts of a "Bravais lattice" and a "reciprocal lattice" are fundamental in the Bloch theory of solids. The vectors of these lattices appear in the theory as purely classical quantities despite the fact that the dynamics of solids has to be treated quantum mechanically.[1]

In this paper we solve two problems. First, we give a quantum-mechanical description of the Bravais and the reciprocal lattices. This consists of finding lattice operators whose eigenvalues are all the discrete vectors of the direct and reciprocal lattices. The eigenfunctions of the lattice operators form a complete orthonormal set of localized functions in both the configuration and the Fourier space.

The second problem is closely related to the first one and has to do with the structure of the kq representation. As was previously shown,[2,3] k and q are the symmetric coordinates for describing dynamics in periodic systems and they assume values in the unit cells of the reciprocal and the direct lattices correspondingly. A natural question to ask is what are the conjugate operators to the ones defining the kq coordinates? Since k and q are periodic coordinators (like angular coordinates) one should expect that their conjugate operators will have discrete eignevalues only. It will be shown in this paper that the above-mentioned lattice operators are conjugate to the operators that define the kq coordinates. Physically, the meaning of the mutually conjugate operators is very simple. The kq coordinates assume values in the unit cells of the reciprocal and direct lattices while the eigenvalues of the lattice operators are the discrete Bravais and reciprocal-lattice vectors.

For simplicity, let us consider the one-dimensional case (the generalization of the results to three dimensions is straightforward). In what follows we show that it is extremely simple to define lattice operators (operators whose eigenvalues are the Bravais and reciprocal-lattice vectors) in the kq coordinates. Suppose that we choose the wave function $C(kq)$ in the kq representation to be periodic in both k and q with the periods $2\pi/a$ and a correspondingly. Then in analogy with the angular coordinate in quantum mechanics[4] the operators conjugate to k and q will be correspondingly

$$i\frac{\partial}{\partial k} \quad \text{and} \quad -i\frac{\partial}{\partial q}. \tag{1}$$

(The choice of sign will become clear from the connection with the x and p operators.) Their eigenfunctions are

$$\varphi_{lm}(kq) = \frac{1}{(2\pi)^{1/2}} \exp\left(i\frac{2\pi}{a}ql - ikam\right), \tag{2}$$

with l and m assuming values from $-\infty$ to $+\infty$. The eigenvalues of the operators (1) are ma and $l(2\pi/a)$, the vectors of the Bravais and reciprocal lattices, correspondingly. (1) are therefore lattice operators and (2) their eigenfunctions (they form a complete set in the periodic space of k and q). In addition, the operators (1) are evidently conjugate to k and q when taken as periodic coordinates.

It would seem that this completes the construction of the lattice operators in the kq representation. However, the following remark shows that this is not so. In defining the kq representation the phases were chosen in such a way as to make any wave function $C(kq)$ to be Bloch-like, namely, $C(kq)$ has to satisfy the following quasiperiodic conditions[2]

$$C[k + (2\pi/a)q] = C(kq), \quad C(kq + a) = e^{ika}C(kq). \tag{3}$$

In the space of Bloch-like function (3) the fundamental operators x and p are[2]

$$x = i\frac{\partial}{\partial k} + q, \quad p = -i\frac{\partial}{\partial q}. \tag{4}$$

The functions $\varphi_{lm}(kq)$ in (2) do not satisfy the quasiperiodicity conditions (3) and they do not therefore belong to the kq space. [One could certainly use a different phase convention which would change both (3) and (4); we find however that the phase choice leading to (3) and (4) is most convenient.]

The functions $\varphi_{lm}(kq)$ in (2) can be made to belong to the kq space by multiplying them by a phase factor $\exp[i\alpha(kq)]$ that satisfies conditions (3).

$$\exp\{i\alpha[k+(2\pi/a)q]\}=e^{i\alpha},$$
$$\exp[i\alpha(kq+a)]=e^{ika}e^{i\alpha}. \tag{5}$$

The functions (2) will become

$$C_{lm}(kq)=\frac{1}{(2\pi)^{1/2}}\exp\left(i\frac{2\pi}{a}ql-ikam+i\alpha(kq)\right). \tag{6}$$

The lattice operators will correspondingly be modified

$$Q=i\frac{\partial}{\partial k}+\frac{\partial\alpha(kq)}{\partial k}, \tag{7}$$
$$K=-i\frac{\partial}{\partial q}-\frac{\partial\alpha(kq)}{\partial q}. \tag{8}$$

Q is the Bravais lattice operator, while K is the reciprocal-lattice operator. The phase $\alpha(kq)$ in relations (6)–(8) has to satisfy the quasiperiodicity conditions (5) and is otherwise arbitrary.

Apart from the arbitrariness in phase $\alpha(kq)$ the construction of the lattice operators Q and K and their eigenfunctions in the kq representation is now completed. Q and K are the lattice operators because their eigenfunctions (6) form a complete set with the eigenvalues ma and $l(2\pi/a)$ correspondingly (m and l assume integer values from $-\infty$ to $+\infty$). In addition Q and K are conjugate to $\exp(ika)$ and $\exp[i(2\pi/a)q]$ correspondingly:

$$[Q,\exp(ika)]=-a\exp(ika),$$
$$\{K,\exp[i(2\pi/a)q]\}=(2\pi/a)\exp[i(2\pi/a)q]. \tag{9}$$

Having the lattice operators Q, K and their eigenfunctions (6) in the kq representation one can find the corresponding results in any other representation, e.g., x and p representation. Thus, the eigenfunctions $\varphi_{lm}(x)$ in the x representation will be[2]

$$\varphi_{lm}(\alpha)=\left(\frac{a}{2\pi}\right)^{1/2}\int_{-\pi/a}^{\pi/a}dk\,C_{lm}(kx). \tag{10}$$

Also, for the lattice operators in the x representation one has

$$\langle x|Q|x'\rangle=\sum_{lm}ma\varphi^{*}_{lm}(x)\varphi_{lm}(x'), \tag{11}$$

$$\langle x|K|x'\rangle=\sum_{lm}l\frac{2\pi}{a}\varphi^{*}_{lm}(x)\varphi_{lm}(x'). \tag{12}$$

Results (10)–(12) are clearly very sensitive to the choice of phase $\alpha(kq)$ in the wave function (6). One should point out that any phase $\alpha(kq)$ satisfying the quasiperiodicity conditions (5) is necessarily a discontinuous function.[5] Let us consider two examples for $\alpha(kq)$. First,

$$\alpha_1(kq)=\bar{k}q,$$

where (13)

$$\bar{k}=k \quad \text{for } -\pi/a<k<\pi/a$$

and $\bar{k}$ is periodic in k with the period $2\pi/a$. $\bar{k}$ can be called a sawlike function of k. For this choice of phase the eigenfunctions in the x representation of the lattice operators Q and K will become [according to formula (10)]

$$\varphi_{lm}(x)=\frac{1}{\sqrt{a}}\exp\left(i\frac{2\pi}{a}xl\right)\frac{\sin(\pi/a)(x-ma)}{(\pi/a)(x-ma)}. \tag{14}$$

For $l=0$ these functions are known as the Wannier functions for the lowest band of a free electron[6] (or an "empty lattice"). It is interesting to point out that for the particular choice of phase in (13) the eigenfunctions (6) with $\alpha_1(kq)$ are closely connected with the Bloch functions for an empty lattice. In the kq representation the latter are[2]

$$C_{lk_B}(kq)=\frac{1}{\sqrt{a}}\exp\left(i\frac{2\pi}{a}ql+i\bar{k}q\right)\delta(k-k_B), \tag{15}$$

where k_B is the conserved Bloch quasimomentum. The function (15) are eigenfunctions of the momentum p [with the eigenvalues $(2\pi/a)l+\bar{k}_B$] and the lattice vector K [with the eigenvalues $(2\pi/a)l$], while the functions (6) are eigenfunctions of both lattice operators Q and K. From point of view of band structure of a free electron it is more convenient to label the functions (15) in such a way as to make l have the meaning of a band index (we shall write them now in the x representation[2] and denote the band index by n). For even n we have

$$\psi_{nk_B}(x)=\begin{cases}\dfrac{1}{(2\pi)^{1/2}}\exp\left(i\dfrac{\pi}{a}nx+i\bar{k}_Bx\right) & \text{for } k_B>0,\\[2ex] \dfrac{1}{(2\pi)^{1/2}}\exp\left(-i\dfrac{\pi}{a}nx+i\bar{k}_Bx\right) & \text{for } k_B<0;\end{cases}$$

and for odd n,

$$\psi_{nk_B}(x)=\begin{cases}\dfrac{1}{(2\pi)^{1/2}}\exp\left(-i\dfrac{\pi}{a}(n+1)x+i\bar{k}_Bx\right) & \\ \quad \text{for } k_B>0,\\[2ex] \dfrac{1}{(2\pi)^{1/2}}\exp\left(i\dfrac{\pi}{a}(n+1)x+i\bar{k}_Bx\right) & \\ \quad \text{for } k_B<0,\end{cases} \tag{16}$$

where n is the band index assuming integer values from 0 to infinity. The choice of the Bloch functions for a free electron in the form (16) makes the band energy $\epsilon_n(k_B)$ a continuous and a periodic function of k_B. The Wannier functions for the Bloch functions (16) are

$$a_n(x-ma)=\frac{1}{\sqrt{a}}\cos\left(\frac{\pi}{a}n+\frac{\pi}{2a}\right)(x-ma)\times\frac{\sin(\pi/2a)(x-ma)}{(\pi/2a)(x-ma)}\quad\text{for even } n,$$
$$a_n(x-ma)=\frac{1}{\sqrt{a}}\cos\left(\frac{\pi}{a}(n+1)+\frac{\pi}{2a}\right)\times(x-ma)\frac{\sin(\pi/2a)(x-ma)}{(\pi/2a)(x-ma)}\quad\text{for odd } n. \tag{17}$$

For $n=0$ we get the same Wannier functions as for $n=0$ in (14). For other values of n the set of Wannier functions for a free electron are closely connected to the eigenfunctions (14) of the lattice operators Q and K. Second,

$$\alpha_2(kq)=k(q-\bar{q}),$$

where (18)

$$\bar{q}=q \quad \text{for } -\tfrac{1}{2}a<q<\tfrac{1}{2}a$$

and $\bar{q}$ is periodic in q with the period a. Let us point out that this choice of phase satisfies conditions (5) because $q-\bar{q}$ assumes only values of the Bravais lattice vectors and $\alpha_2(kq)$ is therefore periodic in k.

eigenfunctions in the x representation of the lattice operators are [according to (10) and (6)]

$$\psi_{lm}(x)=(1/\sqrt{a})\exp[i(2\pi/a)xl]\Theta(x-ma), \tag{19}$$

where

$$\Theta(x)=\begin{cases}1, & -\tfrac{1}{2}a<x<\tfrac{1}{2}a,\\ 0, & \text{otherwise.}\end{cases} \tag{20}$$

While the eigenfunctions (14) were closely connected with the Wannier functions for a free electron, and fell off as $1/x$, the functions (19) correspond to extremely localized Wannier functions which extend over one unit cells and are zero outside the unit cell. One can see that the eigenfunctions (19) are closely connected to the Wannier functions of a tight-binding model with the following periodic potential

$$V(x)=\sum_n U(x-na), \tag{21}$$

where

$$U(x)=\begin{cases}0 & \text{for } x\neq\pm\tfrac{1}{2}a,\\ \infty & \text{for } x=\pm\tfrac{1}{2}a.\end{cases} \tag{22}$$

In the kq representation the functions satisfying the Bloch equation inside each unit cell for the potential (21) are

$$C_{lk_B}(kq)=\frac{1}{\sqrt{a}}\exp\left(i\frac{2\pi}{a}ql+ik_B(q-\bar{q})\right). \tag{23}$$

Since the potential $V(x)$ is infinite at the boundaries of any unit cell the correct Bloch functions can be chosen to vanish at $q=\pm\frac{1}{2}a$ and one gets (we shall write them now in the x representation[2])

$$\psi_{nk_B}(x)=[1/(2\pi)^{1/2}]\sin(2\pi/a)xn\exp[ik_B(x-\bar{x})], \tag{24}$$

with n assuming values from 0 to infinity. The energy spectrum for these functions is completely flat (k_B independent)

$$\epsilon_n(k_B)=[(2\pi/a)n]^2. \tag{25}$$

The Wannier function for the Bloch functions (24) are

$$a_n(x-ma)=(1/\sqrt{a})\sin(2\pi/a)xn\Theta(x-ma) \tag{26}$$

and are closely connected to the eigenfunctions (19) of the lattice operators Q and K.

What we have shown here is that the eigenfunctions of the lattice operators can be chosen to be either closely related to the Wannier functions of a free electron [phase $\alpha_1(kq)$] or to the Wannier functions of an extremely tightly-bound electron [phase $\alpha_2(kq)$]. For a better comparison of these two cases let us write down the eigenfunctions of the lattice operators for the phase $\alpha_1(kq)$ in the momentum representation (p representation). We have

$$\varphi_{lm}(p)=\left(\frac{a}{2\pi}\right)^{1/2}\exp[-i(p/\hbar)am]\eta[p-l\hbar(2\pi/a)], \tag{27}$$

with

$$\eta(p)=\begin{cases}1 & \text{for } -\pi<pa/\hbar<\pi,\\ 0 & \text{otherwise.}\end{cases} \tag{28}$$

This is exactly the form of the eigenfunctions $\psi_{lm}(x)$ for $\alpha_2(kq)$. Similarly, one can show that the functions $\varphi_{lm}(p)$ for the phase $\alpha_2(kq)$ have the same form as $\varphi_{lm}(x)$ have for the phase $\alpha_1(kq)$. What this means is that for the choice of phase $\alpha_1(kq)$ the eigenfunctions of the lattice operators are very well localized in p space but rather poorly localized in x space (with a fall off as $1/x$). On the contrary, the choice $\alpha_2(kq)$ leads to a very good localization of the eigenfunctions in x space [functions (19)] but in p space they fall off as $1/p$.

We have therefore for the first time constructed a set of lattice operators Q and K having as eigenfunctions a complete set of orthonormal functions and as eigenvalues the Bravais and the reciprocal-lattice vectors. The problem of defining quantum-mechanical lattice operators has been an outstanding problem in solid state theory and there have been attempts to find these operators.[7] There are

a number of textbooks where approaches are made to solving this problem, in particular in connection with the Wannier functions.[8] It should be pointed out that in the kq representation the lattice operators Q and K assume their simplest form [(7) and (8)], while in other representations they can be rather complicated [(11) and (12)]. This should be expected because as was shown in this paper [relations (9)] Q and K are conjugate to the k and q coordinates and it is a rule in quantum mechanics that operators and their eigenfunctions assume usually simple expressions in the space of conjugate coordinates (this can be compared with the simplicity of expressing the momentum operator p and its eigenfunctions in the x representation).

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[1]R. Peierls, *Quantum Theory of Solids* (Oxford U. P., London, 1955).

[2]J. Zak, *Solid State Physics*, edited by F. Seitz, D. Turnbull, and H. Ehrenreich (Academic, New York, 1972), Vol. 27.

[3]J. Zak and J. Birman, Phys. Rev. B 10, 1315 (1974).

[4]L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon, London, 1958).

[5]A proof of this statement will be presented in a later publication. The author is grateful to Professor C. Newman of Indiana University for presenting him with a proof of the above statement.

[6]W. Kohn, Phys. Rev. B 7, 4388 (1973).

[7]E. C. McIrvine and A. W. Overhauser, Phys. Rev. 115, 1531 (1959); E. C. McIrvine, *ibid.* 115, 1537 (1959). In the latter reference a possible application of the lattice representation is outlined.

[8]G. H. Wannier, *Elements of Solid State Theory* Cambridge U. P., Cambridge, England, 1960); G. Weinreich, *Solids, Elementary Theory for Advanced Students* (Wiley, New York, 1965).