kq representation in lattice dynamics*

Joshua Zak† and Joseph L. Birman§
Physics Department, New York University, New York, New York 10003
(Received 22 April 1974)

The kq representation is introduced into lattice dynamics. As in electron dynamics it turns out to be useful both conceptually and for calculational purposes. An integral effective-mass-like equation is derived. It is shown to reproduce the well-known results for localized impurities in lattice dynamics. Similarly the kq representation can be introduced into the description of magnons.

Lattice vibrations in solids are most commonly described by giving the deviations of atoms from equilibrium $\vec{u}(\vec{R}_n+\vec{q}_f)$ as a function of the lattice point $\vec{R}_n+\vec{q}_f$, where $\vec{R}_n$ is the position vector of a unit cell and $\vec{q}_f$ is the location of the atom inside the unit cell. In an ideal crystal these deviations are Bloch waves[1] or phonons while in perturbed crystals one usually finds also localized modes,[2] which can sometimes be given conveniently by Wannier functions.[3] The description of the deviations $\vec{u}$ as a function of the radius vector $\vec{R}_n+\vec{q}_f$ of the atom leads to the lattice dynamics in the coordinate representation.

In a recent series of papers[4] the dynamics of electrons in solids was described in the kq representation. It was shown that both conceptually and practically this representation can be useful in solving a great variety of problems.

This article is intended to introduce the kq representation into lattice dynamics. It is shown that the equations of motion assume an integral form in the kq coordinates. As in the electron dynamics, the kq representation facilitates the separation of coordinates in lattice vibrations. In particular, it is used in this paper for rederiving the equations for the lattice-impurity problem.

The idea of the kq representation is based on the use of the quasimomentum $\vec{k}$ and the quasicoordinate $\vec{q}$ instead of the radius vector $\vec{r}$ in describing dynamics in solids.[4] The quasimomentum $\vec{k}$ varies in a unit cell of the reciprocal lattice while the quasicoordinate $\vec{q}$ assumes values inside a unit cell of the Bravais lattice. Together the kq coordinates can be used instead of one variable $\vec{r}$, which assumes values in all the space. Conceptually the kq representation was introduced on the basis of translations in the direct and the reciprocal space and a quantum-mechanical meaning was attached to the kq coordinates. Namely, $\vec{k}$ labels the eigenvalues of translations in direct space while $\vec{q}$ defines the eigenvalues of translations in inverse space. However, at the same time $\vec{k}$ and $\vec{q}$ can be looked at as regular coordinates (like the radius vector $\vec{r}$) on which any function can depend. As such, the kq coordinates can be used in any dynamics, be it classical or quantum mechanical. In particular, any function of the radius vector $\vec{r}$ can be transformed into a function of the kq coordinates. Thus the kq transform $C(\vec{k}\vec{q})$ of any function $\psi(\vec{r})$ (not necessarily a wave function in quantum mechanics) is as follows[4]:

$$\vec{C}(\vec{k}\vec{q})=\frac{1}{\sqrt{V_b}}\sum_{\vec{R}_m} e^{-i\vec{k}\cdot\vec{R}_m}\vec{\psi}(\vec{q}+\vec{R}_m)\,, \tag{1}$$

where V_b is the volume of a unit cell in the reciprocal lattice. In particular, for a displacement $\vec{u}(\vec{R}_n+\vec{q}_f)$, relation (1) will be

$$C(kq_f)=\frac{1}{\sqrt{V_b}}\sum_{\vec{R}_m} e^{-i\vec{k}\cdot\vec{R}_m}u(\vec{q}_f+\vec{R}_m)\,. \tag{2}$$

In lattice dynamics the radius vector $\vec{r}=\vec{R}_n+\vec{q}_f$ is discrete and the quasicoordinate $\vec{q}_f$ assumes discrete values, while for electrons $\vec{q}$ is a continuous variable. In formal expansions of functions, this will be the only difference in using the kq coordinates in electron dynamics and in lattice vibrations. As will be seen below all the relations that are connected with expansions of functions and transformations from one representation to another can be directly carried over from the wave functions for electrons to displacements for vibrations. As an example let us write down the displacement in the kq representation $\vec{C}(\vec{k}\,\vec{q}_f)$ for a Bloch wave (a phonon) with a branch index l and a wave vector $\vec{k}_B$. In the radius vector $\vec{r}=\vec{R}_n+\vec{q}_f$ representation this displacement is

$$\vec{u}_{lk_B}(\vec{R}_n+\vec{g}_f)=(1/\sqrt{V_b})e^{i\vec{k}_B\cdot\vec{R}_n}\vec{v}_{lk_B}(\vec{q}_f)\,, \tag{3}$$

and the corresponding displacement in the kq representation becomes

$$\vec{C}_{lk_B}(\vec{k}\vec{q}_f)=\delta(\vec{k}-\vec{k}_B)\vec{v}_{lk_B}(\vec{q}_f)\,. \tag{4}$$

This is in complete analogy with the Bloch functions in the kq representation for electrons.[4]

Let us now write the equations of motion for the

vibrations in the kq representation. We shall assume in this paper the validity of a harmonic approximation. In the regular coordinates these equations for a general perturbed crystal can be written as follows[2] (where renormalized force constants ϕ are used in order to eliminate the masses):

$$\sum_{\beta n' f'} \phi_{\alpha\beta}(\vec{R}_n+\vec{q}_f,\ \vec{R}_n'+\vec{q}_f')u_\beta(\vec{R}_n'+\vec{q}_f')=\omega^2 u_\alpha(\vec{R}_n+\vec{q}_f). \tag{5}$$

The force constants will in general contain the unperturbed part $\phi^{(0)}$ and a perturbation V caused by a defect or some kind of irregularity in the crystal:

$$\phi_{\alpha\beta}(\vec{R}_n+\vec{q}_f,\ \vec{R}_n'+\vec{q}_f') = \phi^{(0)}_{\alpha\beta}(\vec{R}_n+\vec{q}_f,\ \vec{R}_n'+\vec{q}_f') + V_{\alpha\beta}(R_n+q_f,\ R_n'+q_f') \tag{6}$$

In order to write the equation of motion in the kq representation both the displacements u and the force constant ϕ have to be Fourier transformed according to the inverse relation of (2),

$$\vec{u}(\vec{q}_f+\vec{R}_n)=\frac{1}{\sqrt{V_b}}\int e^{i\vec{k}\cdot\vec{R}_n}\vec{C}(\vec{k}\vec{q}_f)\,d\vec{k}\ . \tag{7}$$

The equations of motion in the kq coordinates become [the force constants ϕ are transformed twice according to (7)]

$$\sum_{\beta f'}\int d\vec{k}'\ \phi_{\alpha\beta}(\vec{k}\vec{q}_f,\ \vec{k}'\vec{q}_f')C_\beta(\vec{k}'\vec{q}_f')=\omega^2 C_\alpha(\vec{k}\vec{q}_f), \tag{8}$$

where

$$\phi_{\alpha\beta}(\vec{k}\vec{q}_f,\ \vec{k}'\vec{q}_f') = \frac{1}{V_b}\sum_{nn'}\phi_{\alpha\beta}(\vec{R}_n+\vec{q}_f,\ \vec{R}_n'+\vec{q}_f')e^{-i\vec{k}\cdot\vec{R}_n+i\vec{k}'\cdot\vec{R}_n'}. \tag{9}$$

Relations (8) are the equations of motion in integral form for the lattice vibrations. For an ideal crystal $\phi_{\alpha\beta}=\phi^{(0)}_{\alpha\beta}$ the latter depends only on the difference of R_n-R_n' and not on each of the vectors $\vec{R}_n,\vec{R}_n'$ separately. We have therefore

$$\phi^{(0)}_{\alpha\beta}(\vec{k}\,\vec{q}_f,\ \vec{k}'\vec{q}_f') = \sum_l \phi^{(0)}_{\alpha\beta}(\vec{R}_l+\vec{q}_f,\ \vec{q}_f')e^{-i\vec{k}\cdot\vec{R}_l}\delta(\vec{k}-\vec{k}') = D^{(0)}_{\alpha\beta}(\vec{k},\vec{q}_f\vec{q}_{f'})\delta(\vec{k}-\vec{k}')\ . \tag{10}$$

The eigenvalue equations (8), will become

$$\sum_{\beta f'} D^{(0)}_{\alpha\beta}(\vec{k},\vec{q}_f\vec{q}_{f'})C_\beta(\vec{k}\,\vec{q}_f')=\omega^2 C_\alpha(\vec{k}\vec{q}_f)\ . \tag{11}$$

As was already mentioned the functions (4) are solutions of Eq. (11) for a branch index l and a wave vector $\vec{k}_B$. Being solutions of Eq. (11) the functions (4) form a complete set and therefore any functions $\vec{C}(\vec{k}\vec{q}_f)$ can be expanded in them. This is of particular importance when the perturbed problem (8) is being solved.

No matter which problem is solved the displacement in the kq coordinates $\vec{C}(\vec{k}\,\vec{q}_f)$ is a Bloch-like function and satisfies therefore the same boundary conditions as Bloch functions do[4]:

$$\vec{C}(\vec{k}\vec{q}_f+\vec{R}_n)=e^{i\vec{k}\cdot\vec{R}_n}\vec{C}(\vec{k}\vec{q}_f)\ , \tag{12}$$

$$\vec{C}(\vec{k}+\vec{K}\vec{q}_f)=\vec{C}(\vec{k}\vec{q}_f)\ . \tag{13}$$

It is therefore possible to expand any function $\vec{C}(\vec{k}\vec{q}_f)$ in the complete set of functions (4) with the result

$$\vec{C}(\vec{k}\vec{q}_f)=\sum_l B_l(\vec{k})\vec{v}_{lk}(\vec{q}_f)\ . \tag{14}$$

The latter expansion is in complete analogy with the one used in electron dynamics. The simplicity of this expansion is that it contains a summation over the branch index only (no integrations over $\vec{k}$). In electron dynamics this expansion turns out to be useful in a variety of problems.[4]

By using (14) and (7) one can arrive at another expansion which was also used in electron dynamics. For this purpose let us expand $B_l(\vec{k})$ and $\vec{v}_{lk}(\vec{q}_f)$,

$$B_l(\vec{k})=\frac{1}{\sqrt{V_b}}\sum_{\vec{R}_n} e^{-i\vec{k}\cdot\vec{R}_n}F_l(\vec{R}_n)\ , \tag{15}$$

$$\vec{v}_{lk}(\vec{q}_f)=\sum_{\vec{R}_m} e^{i\vec{k}\cdot\vec{R}_m}\vec{a}(\vec{q}_f-\vec{R}_m)\ . \tag{16}$$

In (15) and (16) the summation is over the Bravais-lattice vectors. In the last expansion $\vec{a}_l(\vec{q}_f-\vec{R}_m)$ are the localized or the Wannier functions for the vibrations.[3] By putting (14)–(16) into (7) we have

$$\vec{u}(\vec{q}_f+\vec{R}_n)=\sum_{lm}\vec{a}_l(\vec{q}_f-\vec{R}_m)F_l(\vec{R}_n+\vec{R}_m) = \sum_l \vec{v}_{lk}(\vec{q}_f)F_l(\vec{R}_n)\ \text{ with }\ \vec{k}=-i\frac{\partial}{\partial R_n}\ . \tag{17}$$

The last equality is obtained by using the connection between Bloch functions $\vec{v}_{lk}(\vec{q}_f)$ and Wannier functions $\vec{a}_l(\vec{q}_f-\vec{R}_n)$ as given by relation (16). The operator $\vec{v}_{lk}(\vec{q}_f)$ in (17) is given by (16) with $\vec{k}=-i\partial/\partial\vec{R}_n$. Relation (17) is similar to the corresponding one in electron dynamics.

The expansions (14) and (17) are simply Fourier transforms of one another. They were shown to be useful in electron dynamics and here we shall apply them to the impurity problem in lattice

dynamics.

Let us first rewrite the eigenvalue equation (8) by using expansion (14). It will be assumed that the force constants are given by relation (6) and also that the solutions for the eigenvalues $\omega_m^2(\vec{k})$ and eigenvectors $\vec{v}_{mk}(\vec{q}_f)$ of the unperturbed crystal are known. By using expansion (10) and the orthogonality relations for $\vec{v}_{lk}(\vec{q}_f)$,

$$\sum_{\alpha f} v^*_{\alpha mk}(\vec{q}_f) v_{\alpha lk}(\vec{q}_f) = \delta_{lm} , \tag{18}$$

one obtains the following equation for the coefficients $B_n(\vec{k})$:

$$\omega_m^2(\vec{k}) B_m(\vec{k}) + \sum_l \int V_{ml}(\vec{k}\vec{k}') B_l(\vec{k}')\, d\vec{k}' = \omega^2 B_m(\vec{k}), \tag{19}$$

where

$$V_{ml}(\vec{k}\vec{k}') = \frac{1}{V_b} \sum_{\alpha\beta f f' n n'} v^*_{\alpha mk}(\vec{q}_f) e^{-i\vec{k}\cdot\vec{R}_n} V_{\alpha\beta}(\vec{R}_n + \vec{q}_f, \vec{R}'_n + \vec{q}'_{f'}) \times v_{\beta lk'}(\vec{q}'_{f'}) e^{i\vec{k}'\cdot\vec{R}'_n} . \tag{20}$$

Equations (19) are the exact lattice-dynamics equations written in the nk representation (branch-index and wave-vector representation). They form a coupled system of integral equations and they have the structure of effective-mass equations for electrons.[5] The application of these equations to specific problems will be discussed in future work. Here we shall show that Eqs. (19) very simply reproduce the eigenvalue equations for a localized impurity.

In general, relation (20) can be rewritten

$$V_{ml}(\vec{k}\vec{k}') = \sum_{\alpha f n} v^*_{\alpha mk}(\vec{q}_f + \vec{R}_n)\ \ t_{\alpha lk'}(\vec{q}_f + \vec{R}_n) , \tag{21}$$

where

$$t_{\alpha lk'}(\vec{q}_f + \vec{R}_n) = \sum_{\beta f' n'} V_{\alpha\beta}(\vec{R}_n + \vec{q}_f, \vec{R}'_n + \vec{q}'_{f'}) v_{\beta lk'}(\vec{q}_f + \vec{R}'_n). \tag{22}$$

If only nearest neighbors are affected by the impurity then the summation in (21) and (22) is clearly only over those atoms that surround the impurity (including the impurity). By assuming that $\omega^2 \neq \omega_m^2(\vec{k})$ (we are looking only for perturbed modes), it follows from (19) and (21)

$$B_m(\vec{k}) = \frac{\sum_{\alpha f n} v^*_{\alpha mk}(\vec{q}_f + \vec{R}_n) \sum_l \int dk'\, t_{\alpha lk'}(\vec{q}_f + \vec{R}_n) B_l(\vec{k}')}{\omega^2 - \omega_m(\vec{k})} . \tag{23}$$

Now multiply both sides of Eq. (23) by $t_{\beta mk}(\vec{q}'_f + \vec{R}'_n)$, sum over m and integrate over $\vec{k}$. The result is

$$b_\beta(\vec{q}'_f + \vec{R}'_n) = \sum_{\alpha f n} A_{\alpha\beta}(\vec{R}_n + \vec{q}_f, \vec{R}'_n + \vec{q}'_f) b_\alpha(\vec{q}_f + \vec{R}_n), \tag{24}$$

where

$$b_\alpha(\vec{q}_f + \vec{R}_n) = \sum_l \int d\vec{k}\, t_{\alpha lk}(\vec{q}_f + \vec{R}_n) B_l(\vec{k}) \tag{25}$$

and

$$A_{\alpha\beta}(\vec{R}_n + \vec{q}_f, \vec{R}'_n + \vec{q}'_f) = \sum_m \int d\vec{k}\, \frac{v^*_{\alpha mk}(\vec{q}_f + \vec{R}_n) t_{\beta mk}(\vec{q}'_f + \vec{R}'_n)}{\omega^2 - \omega_m^2(\vec{k})} = \sum_m \int d\vec{k} \sum_{\gamma f'' n''} \frac{v^*_{\alpha mk}(\vec{q}_f + \vec{R}_n) V_{\beta\gamma}(\vec{R}'_n + \vec{q}'_f, \vec{R}''_n + \vec{q}''_f) v_{\gamma mk}(\vec{q}''_f + \vec{R}''_n)}{\omega^2 - \omega_m^2(\vec{k})} . \tag{26}$$

Equations (24) are linear homogeneous equations for the impurity modes of the perturbed crystal. They are the same equations as those obtained by the Green's-function technique.[2] The frequencies of the perturbed modes are given by the secular equation

$$\det(A - I) = 0 , \tag{27}$$

where I is a unit matrix and the A matrix is given in (26).

As is well known, Eqs. (24) assume a particularly simple form for an isotopic impurity where an atom with a mass M'_1 replaces the atom with mass M_1 at the lattice point $\vec{R}_n = 0$ and $\vec{q}_f$ with $f = 1$. For this situation the perturbation matrix V becomes[2]

$$V_{\alpha\beta}(\vec{R}_n + \vec{q}_f, R'_n + \vec{q}'_f) = (1 - M'_1/M_1)\omega^2 \delta_{n0}\delta_{n'0}\delta_{f1}\delta_{f'1}\delta_{\alpha\beta} . \tag{28}$$

Relation (21) assumes then a very simple form:

$$V_{ml}(\vec{k}\vec{k}') = (1 - M'_1/M_1)\omega^2 \sum_\alpha v^*_{\alpha mk}(\vec{q}_1) v_{\alpha lk'}(\vec{q}_1) . \tag{29}$$

Correspondingly the matrix A in (26) that defines the eigenvalue equations (24) and the secular equation (27) is a 3×3 matrix,

$$A_{\alpha\beta} = (1 - M_1'/M_1)\omega^2 \sum_m \int d\vec{k}\, \frac{v^*_{\alpha m k}(\vec{q}_1) v_{\beta m k}(\vec{q}_1)}{\omega^2 - \omega_m^2(\vec{k})}. \tag{30}$$

We have therefore shown that the integral equations (19) in the nk representation can be used as starting equations for reproducing the well-known results for localized impurities in lattice dynamics. However, since Eqs. (19) have the structure of the effective-mass equation one should expect that they will be useful in treating extended impurities. Recently this extended-impurity problem has been treated by an effective-mass-equation approach[6,7] and by integral equations of the type (19) but for the Green's function.[8]

An alternative form of Eqs. (19) can be obtained by using expansion (17). This will lead to equations for lattice dynamics in the lR representation, l being the branch index and $\vec{R}$ the Bravais-lattice vector. In order to arrive at the other form of the equations, expansion (17) is substituted into Eqs. (5) (expression (6) will again be assumed for the force constants), the result multiplied from the left by the operator $v^\dagger_{\alpha m k}(\vec{q}_f)$, and everything summed over α and f. Alternatively, the same result can be obtained by Fourier transforming Eqs. (19). One arrives at the following equations in the lR representation (a result that was obtained in Ref. 6):

$$\omega_m^2\left(-i\frac{\partial}{\partial \vec{R}}\right) F_m(\vec{R}) + \sum_l V_{ml}(\vec{R}, \vec{R}') F_l(\vec{R}') = \omega^2 F_m(\vec{R}), \tag{31}$$

where

$$V_{ml}(\vec{R}, \vec{R}') = \frac{1}{V_b} \int d\vec{k}\, d\vec{k}'\, V_{ml}(\vec{k}\vec{k}') e^{\,i\vec{k}\cdot\vec{R} - i\vec{k}'\cdot\vec{R}'}$$
$$= \sum_{\alpha\beta f f' n n'} a^*_{\alpha m}(\vec{q}_f - \vec{R} + \vec{R}_n)$$
$$\times V_{\alpha\beta}(\vec{R}_n + \vec{q}_f, \vec{R}_n' + \vec{q}_f') a_{\beta l}(\vec{q}_f' - \vec{R}' + \vec{R}_n'). \tag{32}$$

In (32) $V_{ml}(\vec{k}\vec{k}')$ is given by relation (20) while $a_{\alpha m}$ and $a_{\beta l}$ are the Wannier functions defined in (16).

One should expect that in some problems of lattice dynamics the eigenvalue equations in the form (19) will be useful while in other problems one will prefer using Eqs. (31).

In conclusion we would like to point out that exactly the same method as in lattice dynamics can be used for introducing the kq representation into the description of magnons.

---

*Supported in part by NSF Grant No. NSF-GH-31742 and AROD Grant AROD-DAH-C04-74-G0109.

†Visiting Professor at New York University, Spring 1974. Permanent address: Physics Department, Technion, Haifa, Israel.

§Address after 1 September 1974: Physics Department, City College of the CUNY, Convent Ave. at 138 St., New York, N.Y. 10031.

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

[2]A. A. Maradudin, *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic, New York, 1966), Vol. 18.

[3]W. Kohn, Phys. Rev. B 7, 2285 (1973).

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

[5]J. M. Luttinger and W. Kohn, Phys. Rev. 97, 869 (1955).

[6]J. L. Birman and P. Pfeuty (unpublished).

[7]V. V. Bryxin and Yu. A. Firsov, Zh. Eksp. Teor. Fiz. 58, 1025 (1970) [Sov. Phys.—JETP 31, 551 (1970)]; Fiz. Tverd. Tela 12, 1030 (1970) [Sov. Phys.—Solid State 12, 809 (1970)]; also, in *Proceedings of the International Seminar "Selected Problems in the Theory of Impurity Centers in Crystals,"* edited by G. Zavt (Academy of Sciences of Estonian SSR, Tallin, 1972).

[8]J. Oitmaa and A. A. Maradudin, Solid State Commun. 7, 1371 (1969).