The Journal of National Chiao Tung University
Vol. 4, April 1978
pp. 57-66

具有緩慢包跡變化之週期位能系統的等效韓彌爾頓理論

Effective Hamiltonian Theory for A Periodic Potential with Slowly Varying Envelop

盧志遠 Chih-Yuan Lu

Institute of Electronics, N. C. T. U.

(Received February 28, 1978)

Abstract — Using kq-representation of quantum mechanics to formulate the problem of an electron moving in a periodic potential with a slowly varying envelop. An explicit equation is derived for the first order, and the higher order terms can be obtained by systematic expansion. The kq-representation is briefly introduced in the Appendix.

It is well known that, in semiconductor physics, the effective mass formula can describe the impurity state very well. This theory was rigorously justified by Luttinger and Kohn. [1] In this case, it is assumed that the potential due to the impurity ion is slowly varying [Fig. 1(a)]. By this assumption, we can use the Luttinger and Kohn effective mass theory to reduce the problem into a very simple form. In this report, I would like to solve another problem which aeems very close to the old problem, but they are different, and I will use a new technique-kq representation [2] to solve this problem. The potentials of this problem are located on regular lattice points but their magnitudes are slowly varying. The situation can be illustrated as Fig. 1 (b).

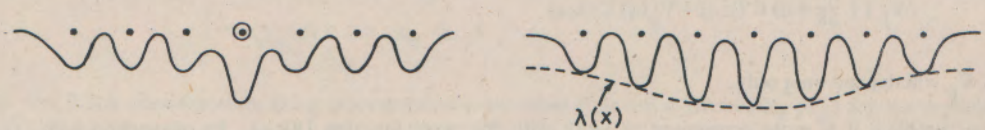

Fig. 1 (a) The potential with an impurity ion located on the lattice point.

(b) The periodic potential with a slowly varying envelop.

For simplicity, we deal with one dimensional case, and it is easy to generalize to three demiensional case. The Hamiltonian of this problem is given by

$$\mathcal{H} = \frac{p^2}{2} + \lambda(x)\, V_p(x) \tag{1}$$

where we take the unit such that $\hbar = m_e = 1$. $V_p(x)$ is a periodic potential with lattice constant a. $\lambda(x)$ is the slowly varying potential, that means over a lattice spacing a, $\lambda(x)$ changes very little.

$$\frac{|\lambda(x+a) - \lambda(x)|}{|\lambda(x)|} \ll 1 \tag{2}$$

We will obtain the effective Hamiltonian theory by introducing the kq-representation, which is explained in Appendix.

The Schrodinger equation we want to solve is

$$[\frac{p^2}{2} + \lambda(x) V_p(x)] \psi(x) = E \psi(x) \tag{3}$$

If the slowly varying envelope function $\lambda(x)$ is a constant λ, the solution is just Bloch states $\psi_{nk}(x)$, that is

$$[\frac{p^2}{2} + \lambda V_p(x)] \psi_{nk}(x) = \epsilon_n(k;\lambda) \psi_{nk}(x)$$

we can express Eq. (3) in kq-representation as follows:

$$\{\tfrac{1}{2}(-i\frac{\partial}{\partial q})^2 + \lambda(i\frac{\partial}{\partial k} + q) V_p(i\frac{\partial}{\partial k} + q)\} C(k,q) = E\, C(k,q) \tag{4}$$

(In kq-representation, we express momentum operator p as $-i\frac{\partial}{\partial q}$; coordinate operator x as $i\frac{\partial}{\partial k} + q$, the detailed explanations are included in Appendix).

The boundary conditions for C(k,q) are:

$$C(k + K_m, q) = C(k,q)$$

$$C(k, q+R_n) = e^{ikR_n} C(k,q)$$

Since $V_p(x)$ is a periodic function of period a, we have

$$V_p(i\frac{\partial}{\partial k} + q) C(k,q) = V_p(q) C(k,q)$$

That is, V_p will depend on q only.

In our problem it is more convenient to work with the wave function U(k,q). Its connection with C(k, q) is given by

$$C(k,q) = e^{ikq} U(k,q)$$

Then the boundary conditions are:

$$\begin{aligned} U(k + K_m, q) &= e^{-iqK_m} U(k,q) \qquad & K_m &= m \cdot (\frac{2\pi}{a}) \\ U(k, q + R_n) &= U(k,q) & R_n &= n \cdot a \end{aligned} \tag{5}$$

And Eq. (4) will become

$$\{\tfrac{1}{2}(-i\frac{\partial}{\partial q} + k)^2 + \lambda(i\frac{\partial}{\partial k}) V_p(q)\} U(k,q) = E\, U(k,q) \tag{6}$$

By the phase transformation (5), the expressions for the basic operators p and x also become

$$p \to -i\frac{\partial}{\partial q} + k$$

$$x \to i\frac{\partial}{\partial k}$$

Therefore, in Eq. (6), the potential term is separated into a product of two terms, one of which depends on q, another depends on $i\frac{\partial}{\partial k}$.

Let us digress to see the representation transformation among the various representations for a periodic system. In x-representation, the equation is given by

$$\{\tfrac{1}{2}(-i\frac{\partial}{\partial x})^2 + \lambda V_p(x)\}\ \psi(x) = E\ \psi(x)$$

its solutions are Bloch functions in x-representation, that are

$$\psi_{nk_B}(x) = e^{ik_B x}\, u_{nk_B}(x),\quad u_{nk_B}(x + \ell\, a) = u_{nk_B}(x)$$

In kq-representation, the periodic Schrodinger equation is

$$\{\tfrac{1}{2}(-i\frac{\partial}{\partial q} + k)^2 + \lambda V_p(q)\}\ U(k,q) = E\ U(k,q) \tag{7}$$

the solutions are given by

$$\begin{aligned} U_{nk_B}(k,q) &= e^{-ikq}\, C_{nk_B}(k,q) = e^{-ikq} \int dx\, \psi_{nk_B}(x)\, \psi_{kq}(x) \\ &= e^{-ikq}\, \psi_{nk_B}(q) \sum_{K_m} \delta(k - k_B - K_m) \\ &= u_{nk_B}(q) \sum_{K_m} \delta(k - k_B - K_m) \end{aligned} \tag{8}$$

If in the Bloch representation (nk_B representation), the wave function is given by $B_n(k_B)$ for the periodic system, this can be obtained by expanding U(k,q) by the Bloch functions in the kq-representation $U_{nk_B}(k,q)$

$$\begin{aligned} U(k,q) &= \sum_{n,k_B} U_{nk_B}(k,q)\, B_n(k_B) \\ &= \sum_{n,k_B} u_{n\,k_B}(q) \sum_{K_m} \delta(k - k_B - K_m)\, B_n(k_B) \\ &= \sum_n B_n(k)\, u_{nk}(q) \end{aligned} \tag{9}$$

In the Bloch representation, Eq. (7) can be written as

$$\epsilon_n(k)\, B_n(k) = E\, B_n(k) \tag{10}$$

and the transformation matrix between the kq-representation and nk_B-representation is given by $U_{nk_B}(k,q)$

$$U(k,q) \xleftrightarrow{U_{nk_B}(k,q)} B_n(k_B)$$

For the non-periodic problem (3), we suggest that it may be possible to just replace the constant λ in the transformation matrix by the slowly varying $\lambda(i\frac{\partial}{\partial k})$ and this matrix will diagonalize Eq. (3) in the band indices. The main idea of an effective Hamiltonian theory is to write Eq. (3) in a Bloch type (nk_B) representation and to keep to some approximation only oneband terms.

Assume a general transformation is performed from the wave function U(k, q) in the kq-representation to the wave function $B_n(k_B)$ in the nk_B-representation:

$$U(k, q) = \sum_{n, k_B} (kq \mid nk_B)\, B_n(k_B) \tag{11}$$

where $(kq \mid nk_B)$ is the transformation matrix. Let us assume that $(kq \mid nk_B)$ form a complete orthonormal set of functions, so that the following relations hold:

$$\int dkdq\, (nk_B \mid kq)(kq \mid n'k'_B) = \delta_{nn'}\, \delta(k_B - k'_B) \tag{12}$$

$$\sum_{n, k_B} (kq \mid nk_B)(nk_B \mid k'q') = \delta(k - k')\ \delta(q - q') \tag{13}$$

Using these properties, the Schrodinger equation (3) can be written in the Bloch (nk_B) representation:

$$\sum_{n', k'_B} H_{nn'}(k_B, k'_B; \lambda)\, B_n(k'_B; \lambda) = E\, B_n(k_B; \lambda) \tag{14}$$

where

$$H_{nn'}(k_B, k'_B; \lambda) = \int dkdq\, (nk_B \mid kq)\, \{ \tfrac{1}{2}(-i \frac{\partial}{\partial q} + k)^2 + \lambda (i \frac{\partial}{\partial k}) V_p(q) \} (kq \mid n'k'_B) \tag{15}$$

From the above discussions, we know that if $\lambda (i \frac{\partial}{\partial k})$ is just a constant λ, then the $(nk_B \mid kq)$ are $U_{nk_B}(k, q)$ given by the Eq. (8)

$$(nk_B \mid kq) = u_{nk}(q; \lambda) \sum_{K_m} \delta(k - k_B - K_m)$$

which can diagonalize the periodic Schrodinger equation. Therefore, we suggest that Eq. (14) perhaps could be diagonalized by the matrices $u_{nk}(q; \lambda \to \lambda(i \frac{\partial}{\partial k})) \sum_{K_m} \delta(k - k_B - K_m)$. The problem is that these matrices are not well defined, because of the non-commutative property of k and $i \frac{\partial}{\partial k}$.

One possible way to obtain the well-defined operator $S(k; \lambda(i \frac{\partial}{\partial k}))$ from $S(k; \lambda)$ is to symmetrize all the products of k and λ of $S(k; \lambda)$ and then replace λ by $\lambda(i \frac{\partial}{\partial k})$. The functions $S(k; \lambda(i \frac{\partial}{\partial k}))$ obtained by such a procedure will be denoted by square bracket: e.g., $[S(k; \lambda)]$. Now let us prescribe the product rule for $[A(k; \lambda)]$ $[B(k; \lambda)]$. One way to symmetrize to products of k and λ in $A(k; \lambda)$ is to express $A(k; \lambda)$ in the following way:

$$A(k; \lambda) = \int dxdy\, \tilde{A}(x, y)\, e^{ikx + i\lambda y}$$

Therefore, $[A(k; \lambda)]$ is given by

$$[A(k; \lambda)] = \int dxdy\, \tilde{A}(x, y)\, e^{ikx + i\lambda(i \frac{\partial}{\partial k})y}$$

If λ is formally small, then $[k, \lambda(i \frac{\partial}{\partial k})] = -i \frac{\partial}{\partial k} \lambda(R) \equiv 2i\eta$ by the properties of small magnitude and slowly varying of $\lambda(x)$, η will be even smaller and slower varying. Also we use the operator identity

$$e^A e^B = e^{A + B + \frac{1}{2}[A, B]}$$

Hence, the product can be written as:

$$[A(k;\lambda)]\,[B(k;\lambda)]$$

$$= \int dxdy\, \tilde{A}(x,y)\, e^{ikx + i\lambda y} \int dudv\, \tilde{B}(u,v)\, e^{iku + i\lambda v}$$

$$= \int dxdydudv\, \tilde{A}\tilde{B}\, e^{\,i(kx+\lambda y + ku + \lambda v) + \frac{i}{2}[kx+\lambda y,\, ku+\lambda v]}$$

where

$$[kx + \lambda y,\, ku + \lambda v] = 2i\eta \cdot (xv - yu)$$

so

$$[A(k;\lambda)]\,[B(k;\lambda)]$$

$$= \int dxdydudv\, \tilde{A} \cdot \tilde{B}\, e^{-\eta(xv-yu)} \cdot e^{i(kx+\lambda y+ku+\lambda v)}$$

$$= \int dxdydudv\, \tilde{A} \cdot \tilde{B}\, e^{-\eta\{(\frac{1}{i}\frac{\partial}{\partial k})(\frac{1}{i}\frac{\partial}{\partial \lambda'}) - (\frac{1}{i}\frac{\partial}{\partial \lambda})(\frac{1}{i}\frac{\partial}{\partial k'})\}}\, e^{i(kx+\lambda y+ku+\lambda v)}$$

$$= e^{-\eta\{(\frac{1}{i}\frac{\partial}{\partial k})(\frac{1}{i}\frac{\partial}{\partial \lambda'}) - (\frac{1}{i}\frac{\partial}{\partial \lambda})(\frac{1}{i}\frac{\partial}{\partial k'})\}}\, (A(k;\lambda)\,B(k';\lambda'))\Big|_{\substack{k=k'\\ \lambda=\lambda'}} \qquad \lambda \to \lambda\,(i\frac{\partial}{\partial k})$$

This means that if we write

$$[C(k;\lambda)] = [A(k;\lambda)]\,[B(k;\lambda)]$$

then $C(k;\lambda)$ is given by

$$C(k;\lambda) = e^{\eta\{\frac{\partial}{\partial k}\frac{\partial}{\partial \lambda'} - \frac{\partial}{\partial k'}\frac{\partial}{\partial \lambda}\}}\, A(k,\lambda)\,B(k',\lambda')\Big|_{\substack{k=k'\\ \lambda=\lambda'}}$$

Therefore

$$[A(k;\lambda)]\,[B(k;\lambda)] = [A(k;\lambda)\,B(k;\lambda)]$$

$$+ \eta\,[\frac{\partial A}{\partial k}\frac{\partial B}{\partial \lambda} - \frac{\partial A}{\partial \lambda}\frac{\partial B}{\partial k}] + \tfrac{1}{2}\eta^2[\,\cdots\,] + \cdots$$

with this product rule, it is easy to see that the matrices

$$(kq\,|\,nk_B)_\lambda = [u_{nk}(q;\lambda)] \sum_{K_m} \delta(k - k_B - K_m)$$

can diagonalize, to the lowest order in η, Eq. (14). To see this, we write Eq. (15) as

$$H_{nn'}(k_B, k'_B) = \int dq\, [u^*_{nk_B}(q;\lambda)]\,[H(k_B, q;\lambda)]\,[u_{n'k_B}(q;\lambda)] \sum_{K_m} \delta(k_B - k'_B - K_m)$$

$$\simeq \delta_{nn'} \int dq \left[u^*_{nk_B}(q;\lambda)\, H(k_B, q;\lambda)\, U_{nk_B}(q;\lambda) \right] \sum_{K_m} \delta(k_B - k'_B - K_m)$$

$$= \delta_{nn'} \left[\epsilon_n(k_B;\lambda) \right] \sum_{K_m} \delta(k_B - k'_B - K_m) \tag{16}$$

Putting Eq. (16) into Eq. (15), we will have the effective Hamiltonian equation to the lowest order in η

$$\left[\epsilon_n(k_B;\lambda) \right] B_n(k_B;\lambda) = E\, B_n(k_B;\lambda) \tag{17}$$

For higher order corrections, the procedure is straightforward but tedious.

Let $\lambda(x)$ be normalized to unity at maximum (at the origin) and of width b ($b \gg a$), we write

$$\lambda(x)\, V_p(x) = V_p(x) + V_p(x)\,(\lambda(x) - 1)$$

therefore, the Schrodinger equation is given by

$$\left[\frac{p^2}{2} + V_p(x) + V_p(x)\,(\lambda(x) - 1) \right] \psi(x) = E\, \psi(x)$$

To see some general features of a simple case, that of weak potential, we use the previous result of the effective Hamiltonian theory in first order to solve the problem. For the low-lying level, we can write the effective Hamiltonian equation (17) as

$$\left[E_b + \frac{p^2}{2m^*} + (\lambda(x) - 1)\, \bar{V}_p \right] \psi = E\, \psi \tag{19}$$

$$\left[\frac{p^2}{2m^*} + (\lambda(x) - 1)\, \bar{V}_p \right] \psi = (\Delta E)\, \psi \tag{20}$$

where m^* is the effective mass of the regular lattice Hamiltonian pant $(m^* = (\partial^2 \epsilon^{(0)}(k)/\partial k^2)^{-1}$ and $\Delta E = E - E_b$, E_b is the band bottom energy. $\bar{V}_p$ is the diagonal matrix element of the unperturbed state.

The example of such a system is a crystal subject to an inhomogeneous strain, the strain makes the crystal potentials distorted continuously, therefore, the Hamiltonian given by equ. (1) should be a simple and reasonable model for this system. As we should have all the informations of the corresponding periodic crystal, therefore, the effective mass of the periodic crystal, the band bottom energy are given, in this way, using our result equ. (20), we can get the low-lying spectrum of this distorted system.

Appendix kq-Representation in the Dynamics of Electrons in Solid

In 1968, J. Zak [2] introduced a new quantum mechanical representation of finite translations and their connection with Bloch functions and Wannier functions. The new representation is used for describing the motion of an electron in a periodic lattice and constant magnetic or electric field. In 1970 [2], he also applied this to the impurity problem in semi-conductors. This representation gives the well-known result of the dynamics of electrons in a solid in a very simple and natural way. The use of the kq-representation leads to a definition of a complete and orthonormal set of functions. These functions are used in developing the effective Hamiltonian theory, and making the effective Hamiltonian theory very transparent and straightforward.

Let us review the main idea and techniques of the kq-representation. For reasons of simplicity, we start with

one dimensional case, and let x and p be the coordinate and momentum that satisfy the commutation relation

$$[\,x, p\,] = i$$

It is known that for a spinless particle either the set of operators x or the set of operators p form a complete set of commuting operators.

Let us now define an operator

$$T(a) = e^{ipa} \qquad (A-1)$$

This operator represents a finite translation in x-space, i.e.,

$$T(a)\ \psi(x) = \psi(x+a)$$

The operators of Eq.(A-1) for a and any multiple of a where a is the lattice constant, are of very great importance in solid state physics. Their importance comes from the fact that they commute with the Hamiltonian for a periodic potential, the period being the lattice length. In order to form a complete set of functions, for example, by Bloch's theorem, we require that the solution of the periodic Schrodinger equation is "also" an eigenfunction of the operator T(a):

$$T(a)\ \psi_k(x) = e^{ika}\ \psi_k(x) \qquad (A-2)$$

Here k specifies the eigenvalues of the translation operator T(a), and k assumes value from $-\frac{\pi}{a}$ to $+\frac{\pi}{a}$. It is clear that (A - 2) itself does not define the function $\psi_k(x)$ completely; it only requires that $\psi_k(x)$ has the form of a Bloch function:

$$\psi_k(x) = e^{ikx}\, u_k(x)$$

where $u_k(x)$ is periodic in x with period a. The operator T(a) by itself does not enough form a complete set of commuting operators (in the way that x or p does), because, as will be shown below, another operator can be found that commutes with T(a), and is not a function of it.

One way of defining the function $\psi_k(x)$ "completely" is to require that $\psi_k(x)$ must satisfy Schrodinger equation. The function $\psi_k(x)$ will now have another quantum number n (band index) to specify the energy eigenvalues completely, that is

$$\psi_{nk}(x) = e^{ikx}\, u_{nk}(x)$$

This is the way Bloch functions are specified by means of a continuous variable k which comes from translation symmetry and a discrete energy band index n. Another way of defining $\psi_k(x)$ in Eq. (A - 2) "completely" is to find other operators that commute with T(a) and that form together with T(a) a complete set. Physically, this means that along with k, one can specify the motion of the electron by another coordinate. Therefore, in order to define $\psi_k(x)$ completely, one has to require that $\psi_k(x)$ is also an eigenfunction of other operators that commute with T(a) and that are independent of T(a). As can be seen an operator that satisfies this requirement is [2]

$$\tau\,(2\,\pi/a) = e^{ix\,\cdot\,\frac{2\pi}{a}} \qquad \text{(A - 3)}$$

The eigenvalues of this operator are $e^{iq\,\frac{2\pi}{a}}$, where q varies from 0 to a. It is clear that the quasi-coordinate is q, and τ is a translation operator in p-space ($\because x = i\,\frac{\partial}{\partial p}$). $\tau\,(\frac{2\pi}{a})$ and T(a) together form "a complete set of commuting operators" or "a quantum mechanical representation".

If we require that the function $\psi_k(x)$ in Eq. (A - 2) is also an eigenfuction of $\tau\,(2\,\pi/a)$, this will define $\psi_k(x)$ "completely". That is,

$$\tau(2\,\pi/a)\,\psi_{kq}(x) = e^{iq\frac{2\pi}{a}}\cdot\psi_{kq}(x)$$

and this requirement leads to the function

$$< x|kq> = \psi_{kq}(x) = (2\,\pi/a)^{-1/2} \sum_n e^{ikna}\ \delta\,(x - q - na) \qquad \text{(A - 4)}$$

The orthogonality relation is given by

$$\int \psi^*_{kq}(x)\ \psi_{k'q'}(x)dx = \sum_m \delta(k - k' - (2\,\pi/a)m) \sum_n \delta(q - q' - na)$$

The completeness is given by

$$\int_{\text{unit cell}} dk \int_{\text{unit cell}} dq\ \ \psi^*_{kq}(x)\ \psi_{kq}(x') = \delta\,(x - x')$$

The functions of eq. (A - 4) are clearly Bloch-like function because they satisfy Eq.(A-2).

It is interesting to compare the kq-representation functions $\psi_{kq}(x)$ in Eq. (A - 4) with the Bloch state functions $\psi_{nk}(x)$ by means of Wannier functions $a_n(x - la)$. Bloch states are given by

$$\psi_{nk}(x) = \sum_\ell e^{ik\ell\,a}\,a_n\,(x - \ell a) \qquad \text{(A - 5)}$$

Comparing Eq.(A-5) with Eq.(A-4),it can be seen that the $\psi_{kq}(x)$ functions are Bloch-type functions corresponding to infinitely-localized Wannier functions. It is easy to get ψ_{kq} in the p representation by taking the Fourier transform of Eq. (A - 4). We get

$$<p\,|\,kq> = \psi_{kq}(p) = \frac{1}{\sqrt{a}}\,e^{-\,ikq} \sum_n \delta(p - k - n\,\frac{2\,\pi}{a})\,\cdot\,e^{iq\,\cdot\,n\,\frac{2\pi}{a}} \qquad \text{(A - 6)}$$

Finally, the eigenfunctions of T(a) and $\tau\,(2\,\pi/a)$ can be written in their own kq-representation:

$$<kq\,|\,k'q'> = \psi_{k'q'}(kq) = \delta\,(k - k')\,\delta\,(q - q') \qquad \text{(A - 7)}$$

In order to be able to write down the Schrodinger eq. in this kq-representation, we need the expressions for the operators x and p in the coordinates k and q. One ahs to calculate the matrices $<k'q'\,|\,x|\,kq>$ and $<k'q'\,|\,p\,|\,kq>$

$$<kq|\,p\,|\,k'q'> = \int dp \int dp' <kq\,|\,p><p|p'><p'\,|\,k'q'>$$

$$= \int dp \langle kq|p\rangle p \langle p|k'q'\rangle = -i \frac{\partial}{\partial q}, \ \delta(q'-q)\,\delta(k'-k) \qquad (A-8)$$

Where we have used expression (A - 6) and similarly, for the operator x,

$$\langle k'q'|x|kq\rangle = i \frac{\partial}{\partial k}, \ \delta(k'-k)\,\delta(q'-q) + q'\,\delta(k'-k)\,\delta(q'-q) \qquad (A-9)$$

This means,

$$p = -i \frac{\partial}{\partial q} \qquad (A-10)$$

$$x = i\left(\frac{\partial}{\partial k}\right) + q \qquad (A-11)$$

This completes the construction of the kq-representation: We have a complete set of commuting operators T and τ, their eigenfunctions Eq. (A - 5), or Eq. (A - 6) or Eq. (A - 7) which form a complete set of eigenfunctions, and we also have expressions for the basis operators x and p.

Let us use the kq-representation to write down the equation for an electron in a periodic lattice and constant magnetic and/or electric field. In doing so, we start with Schrodinger's equation for this problem in the $\vec{r}$-representation:

$$[(\vec{p} + \frac{e}{2c}\vec{H} \times \vec{r})^2/2 + V(\vec{r}) + e\vec{E}\cdot\vec{r}\,]\,\psi(\vec{r}) = \epsilon\,\psi(\vec{r}) \qquad (A-12)$$

where $V(\vec{r})$ is the periodic potential, $\vec{H}$ and $\vec{E}$ are the magnetic and electric field, respectively, and e is the charge of the electron with minus sign (e > 0). By using the three-dimensional version of the expressions (A - 10) and (A - 11), this equation (A - 12) can be written in the kq-representation:

$$\{[-i\frac{\partial}{\partial \vec{q}} + \frac{e}{2C}\vec{H} \times (i\frac{\partial}{\partial \vec{k}} + \vec{q})\,]^2/2 + V(\vec{q}) + e\vec{E}\cdot(i\frac{\partial}{\partial \vec{k}} + \vec{q})\}\,C(kq) = \epsilon\,C(kq) \qquad (A-13)$$

where C (kq) is the wave function in the kq-representation. That the periodic potential is just a function of $\vec{q}$ follows from its periodicity which enables us to use the expansion

$$V(\vec{r}) = \sum_{\vec{K}_m} V(\vec{K}_m)\, e^{i\vec{K}_m\cdot\vec{r}} \qquad (A-14)$$

where $\vec{K}_m$ are vectors of the reciprocal lattice defined by $\vec{K}_m = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3$ and $\vec{a}_i\cdot\vec{b}_j = 2\pi\delta_{ij}$. Expression (A - 14) contains the operator $\tau(\vec{K}_m)$ and since C (kq) must satisfy the relation (A - 17) below, the exponential in Eq.(A - 14) can be replaced by exp $(i\vec{K}_m\cdot\vec{q})$ which leads to $V(\vec{q})$. This makes the kq-representation particularly useful for treating problems with a periodic potential.

The wave function C (kq) is connected to $\psi(\vec{r})$ by the relation

$$\psi(\vec{r}) = \langle\vec{r}|\psi\rangle = \int_{\text{cell}} d\vec{k}\, d\vec{q} \langle kq|\psi\rangle\langle\vec{r}|kq\rangle$$

$$= \int_{\text{cell}} dk\,dq\, C(kq)\ \psi_{kq}(r)$$

where $\psi_{kq}(\vec{r})$ are the eigenfunctions in three-dimension.

$$\psi_{kq}(\vec{r}) = \left[\frac{V_c}{(2\pi)^3}\right]^{1/2} \sum_{\vec{R}_n} \delta(\vec{r} - \vec{q} - \vec{R}_n) \exp(i\vec{k} \cdot \vec{R}_n) \tag{A - 15}$$

V_c is the volume of a unit cell in the direct space. The inverted formula is

$$C(kq) = \int d\vec{r}\ \psi(\vec{r})\ \psi^*_{kq}(\vec{r}) \tag{A - 16}$$

From the Eq. (A - 15) for ψ_{kq}, it follows that C (kq) satisfies the following conditions:

$$C(k + K_m, q) = C(k, q) \tag{A - 17}$$

$$C(k, q + R_n) = e^{ik \cdot R_n} C(k, q) \tag{A - 18}$$

These are the boundary conditions on $C(\vec{k}, \vec{q})$ and we see that the latter conditions (A - 18) are Bloch-type functions. They are periodic in $\vec{k}$, and produce a phase factor $\exp(i\vec{k} \cdot \vec{R}_n)$ when $\vec{q}$ is replaced by $\vec{q} + \vec{R}_n$.

Eq. (A - 13) contains six independent variables $\vec{k}$ and $\vec{q}$. This does not mean that the number of degrees of freedom of the problem has changed. The only thing that happened is that instead of having three variables $\vec{r}$ in an infinite region, we have now six variables $\vec{k}$, $\vec{q}$ that are restricted to unit cells in $\vec{k}$ and $\vec{q}$ spaces. This change leads to a very important consequence. While in Eq. (A - 12), there are terms of infinte magnitude caused by the magnetic and electric fields when $\vec{r} \to \infty$, no such terms appear in Eq. (A - 13) because $\vec{k}$ and $\vec{q}$ are limited to unit cells only.

References

1. J. M. Luttinger and W. Kohn, "Motions of electrons and holes in perturbed periodic fields", Phys. Rev., 97, 869 (1955).
2. J. Zak, "Dynamics of Electrons in Solids in External Fields", Phys. Rev., 168, 686 (1968), "Dyamics of Electrons in Solids in External Fields II ", Phys. Rev., 177, 1151 (1969), "kq-Representation for the Impurity Problem in Semiconductors", Phys. Rev., B2, 384 (1970).