сообщения
объединенного
института
ядерных
исследований
дубна

E17-82-207

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ONE VARIABLE ANALYTICITY AND PERIODICITY OF THE QUASI-BLOCH FUNCTIONS

1982

1. INTRODUCTION

In a classic paper[1], Kohn proved that for one-dimensional crystals, the Bloch functions (i.e., the eigenstates of an electron in a periodic potential) are analytic and periodic functions of the crystal momentum k in a strip of the complex k plane. The generalization of this result to three-dimensional crystals seems to be quite difficult. Des Cloizeaux[2] succeded in the proof of analycity and periodicity properties of Bloch functions of $\vec{k}(\vec{k}=(k_1,k_2,k_3))$ in a strip of the complex $\vec{k}$ plane, under the following circumstances: i. The band is nondegenerated and the crystal has a center of inversion. ii. The tight-binding limit is assumed.

The main interest in proving that the Bloch functions are analytic and periodic functions of $\vec{k}$ consists in the fact that this implies, via the Paley-Wiener theorem, the existence of exponentially localized Wannier functions. However, it is also interesting to prove the analyticity and periodicity of the Bloch functions with respect to only one (two) components of the quasi-impuls, the others being fixed. The reason is that when an external homogeneous electric (magnetic) field is applied, two (one) components of $\vec{k}$ still remain constants of motion.

The main result of this paper is the proof of the existence of quasi-Bloch functions[2,3], analytic and periodic in k_1 at k_2, k_3 fixed, for general crystals (with or without a center of inversion) and degenerated bands. This result is one of the main ingrediants in our proof.[4] concerning the existence of Stark-Wannier resonances[5] of the Bloch electrons in homogeneous electric field. A useful representation for the position operator is also given.

2. THE CONSTRUCTION OF QUASI-BLOCH FUNCTIONS

The Hamiltonian to be discussed is

$$H_0 = -\Delta + V_{per.} \tag{2.1}$$

As for the periodic potential, we shall assume that it is local and square integrable over the unit cell.

Let $\{\vec{a}_i\}_{i=1}^{3}$ be a basis in $\mathbf{R}^3$ and $\{\vec{K}_i\}_{i=1}^{3}$ be the dual basis, i.e.,

$$\vec{a}_i \vec{K}_j = 2\pi\delta_{ij} .$$

Without loss of generality, we shall take the length of $\vec{K}_1$ to be 2π. Let Q be the basic period cell for the basis $\{\vec{a}_i\}$ and B be the basic period cell for $\{\vec{K}_i\}$ (the Brillouin zone). The fact that $|\vec{K}_1| = 2\pi$ means that the length of the Brillouin zone along the $\vec{K}_1$ direction is 2π.

Theorem 1 [6]

Let V be a real function on $\mathbf{R}^3$ with

$$V(\vec{x} + \vec{a}_i) = V(\vec{x}); \quad i = 1,2,3. \tag{2.2}$$

Let

$$\mathcal{H}' = \ell^2(\mathbf{Z}^3) = \{\{\psi_{m_1,m_2,m_3}\} \mid \sum_{m_1,m_2,m_3=-\infty}^{+\infty} |\psi_{m_1,m_2,m_3}|^2 < \infty\}, \tag{2.3}$$

and

$$\mathcal{H} = \int_B^{\oplus} \mathcal{H}' d\vec{k} . \tag{2.4}$$

Suppose $V \in L^2(Q)$ and $\hat{V}_{\vec{m}}$ $(\vec{m} = (m_1, m_2, m_3))$ be the Fourier coefficients of V as a function on Q, i.e., for $\vec{m} \in \mathbf{Z}^3$

$$\hat{V}_{\vec{m}} = (\mathrm{vol.}\, Q)^{-1} \int_Q \exp(-i \sum_{j=1}^{3} m_j \vec{K}_j \vec{x})\, V(\vec{x})\, d\vec{x} . \tag{2.5}$$

For $\vec{k} \in \mathbf{C}^3$, define the operator $H_0(\vec{k})$ in $\mathcal{H}'$ by

$$(H_0(\vec{k})\psi)_{\vec{m}} = (\vec{k} + \sum_{j=1}^{3} m_j \vec{K}_j)^2 \psi_{\vec{m}} + \sum_{\vec{n} \in \mathbf{Z}^3} \hat{V}_{\vec{n}} \psi_{\vec{m}-\vec{n}} , \tag{2.6}$$

with the domain

$$D(H_0(\vec{k})) = D_0 = \{\psi \in \mathcal{H}' \mid \sum_{\vec{m} \in \mathbf{Z}^3} |\vec{m}|^2 \, |\psi_{\vec{m}}|^2 < \infty\} .$$

Then:

i. For $\vec{k} \in \mathbf{R}^3$, $H_0(\vec{k})$ is self-adjoint.

ii. $H_0(\vec{k})$ is an entire analytic family of type A.

iii. For $\vec{k} \in \mathbf{C}^3$, $H_0(\vec{k})$ has compact resolvent.

iv. Let $U: L^2(\mathbf{R}^3, d\vec{x}) \to \mathcal{H}$ be given by

$$(Uf)_{\vec{m}}(\vec{k}) = \hat{f}(\vec{k} + \sum_{j=1}^{3} m_j \vec{K}_j); \quad \vec{k} \in B. \tag{2.7}$$

Then U is unitary, and

$$U H_0 U^{-1} = \int_B^{\oplus} H_0(\vec{k})\, d\vec{k} . \tag{2.8}$$

Proof. For the proof of this theorem, see [6].

In what follows, k_1, k_2, k_3 denote the coordinates of $\vec{k}$ with respect to the basis $\vec{K}_i/|\vec{K}_i|$. We are interested in the properties of $H_0(\vec{k})$ as a function of k_1 at $\vec{k}_\perp = (k_2, k_3)$ fixed. In order to emphasize this fact, we shall write

$$H_0(k_1, \vec{k}_\perp) \equiv H_{0,\vec{k}_\perp}(k_1)$$

and, moreover, in the cases when no confusion is possible, we shall $\vec{k}_\perp$ omit.

Let $\sigma(k_1)$ be the (discrete) spectrum of $H_0(k_1)$.

Definition. A nonvoid part $\sigma^\circ(k_1)$ of $\sigma(k_1)$, $k_1 \in [0, 2\pi]$ is said to be an isolated band of $H_0(k_1)$ if there exist continuous functions on $[0, 2\pi]$, $f_1(k_1)$, $f_2(k_1)$ and a positive constant $c > 0$, such that

$$-\infty < f_1(k_1) < f_2(k_1) < \infty,$$

$$\sigma^\circ(k_1) \subset [f_1(k_1), f_2(k_1)],$$

$$[f_i(k_1) - c, f_i(k_1) + c] \cap \sigma(k_1) = \emptyset, \quad i = 1,2$$

$$k_1 \in [0, 2\pi] .$$

From the physical textbooks, one can learn that, at least for nondegenerated bands, $\sigma^\circ(k_1)$ is the restriction of a periodic function. The precise statement (which is probably a folk-lore, but we do not know a proper reference) is the following.

Let J_d be the strip $|\mathrm{Im}\,k_1| < d$, $\mathrm{Re}\,k_1 \in \mathbf{R}$.

Proposition 1. Let $\sigma^\circ_{\vec{k}_\perp}(k_1)$ be an isolated band of $H_{0,\vec{k}_\perp}(k_1)$. Then:

i. There exist positive integers m, p ; $p \leq m$; functions $\lambda_j(k_1)$, $j = 1,2,\dots,p$ analytic in the strip J_d and real for $k_1 \in \mathbf{R}$; positive integers $r_1,\dots,r_p$ satisfying $\sum_{i=1}^{p} r_i = m$, such that

$$\sigma^\circ_{\vec{k}_\perp}(k_1) = \{\lambda_i(k_1)\}_{i=1}^{p}, \quad k_1 \in [0, 2\pi]$$

each $\lambda_i(k_1)$ having the multiplicity r_i.

ii. The set $\{\lambda_i(k_1)\}_{i=1}^{p}$ is periodic, with period 2π, and each $\lambda_i(k_1)$ is periodic with a period at most $2\pi p$.

Remarks. 1. Note that the existence of some points for which two or more of the functions $\lambda_i(k_1)$ have the same value (intersection or degeneracy points) is allowed. The number of degeneracy points in $[0, 2\pi]$ is finite due to the analyticity properties.

Proof. Let $V: \mathcal{H}' \to \mathcal{H}'$ be the unitary operator given by

$$(V\psi)_{m_1,m_2,m_3} = \psi_{m_1-1,m_2,m_3}. \tag{2.9}$$

Since V is unitary and 1 is not an eigenvalue of V, there exists a unique self-adjoint operator M, such that $\|M\| \leq 1$ and

$$V = \exp(2\pi i M). \tag{2.10}$$

The bounded operator valued function

$$V(k_1) = \exp(ik_1 M), \quad k_1 \in \mathbf{C}, \tag{2.11}$$

is obviously an entire function.

Consider the following family of operators

$$K_{0,\vec{k}_\perp}(k_1) = V(k_1) H_{0,\vec{k}_\perp}(k_1) V^{-1}(k_1). \tag{2.12}$$

A simple, but a little bit tedious calculation shows that

$$K_{0,\vec{k}_\perp}(k_1) = K_{0,\vec{k}_\perp}(k_1 + 2\pi). \tag{2.13}$$

Since $K_{0,\vec{k}_\perp}(k_1)$ and $H_{0,\vec{k}_\perp}(k_1)$ are unitary equivalent, they have the same spectrum and then $\sigma(k_1) \equiv \sigma(H_{0,\vec{k}_\perp}(k_1))$ as a set, is periodic, i.e.,

$$\sigma(k_1) = \sigma(k_1 + 2\pi). \tag{2.14}$$

Defining $\sigma^\circ(k_1)$ for all $k_1 \in \mathbf{R}$ by periodicity, it follows that $\sigma^\circ(k_1)$ is isolated for all $k_1 \in \mathbf{R}$ and $\mathrm{dist.}(\sigma^\circ(k_1), \sigma(k_1) \setminus \sigma^\circ(k_1)) \geq c > 0$, all $k_1 \in \mathbf{R}$. Now, the existence of $\lambda_i(k_1)$, as well as their analyticity properties, follows from the theory of perturbation for analytic families of type A [6]. In particular, the analyticity of $\lambda_i(k_1)$ at degeneracy points, follows from the famous Rellich theorem [6, 7]. The only thing, we have to verify, is the periodicity properties.

As an isolated part of $\sigma(k_1)$, $\sigma^\circ(k_1)$ is a periodic set. Since, because of the analyticity, the number of intersection points in every compact is finite, without loss of generality, we can assume that 0 is not an intersection point. Clearly, if t_i is a smallest integer such that $\lambda_i(2\pi t_i) = \lambda_i(0)$, then the period of $\lambda_i(k_1)$ is $2\pi t_i$. Since for all integers t the set $\sigma^\circ(2\pi t)$ of possible values of $\lambda_i(2\pi t)$ does not depend on t and contains p points, it follows that $t_i \leq p$, and the proof is completed.

Lemma 1. Let $\mathcal{K}$ be a separable Hilbert space and $J_d = \{z \in \mathbf{C} \mid |\mathrm{Im}\,z| < d,\ d > 0\}$. Let $\Pi(z)$ be a projection-valued analytic function in J_d satisfying:

i. $\Pi(z) = \Pi^*(z)$, $z \in \mathbf{R}$.

ii. $\Pi(z) = \Pi(z + 2\pi)$, $z \in J_d$.

Then, there exists an analytic family $A(z)$ of invertible operators with the properties:

a. $A(z)\Pi(0)A^{-1}(z) = \Pi(z)$, $A(0) = 1$.

b. $A^*(z) = A^{-1}(z)$, $z \in \mathbf{R}$.

c. $A(z + 2\pi) = A(z)$, $z \in J_d$.

Remarks. 2. Without the periodicity conditions, the above result goes back to Sz.-Nagy [8] (see also refs. [6,7]). For finite-dimensional Hilbert spaces, related results concerning the periodic case are given in ref. [9] with completely different proofs.

Proof. We shall construct $A(z)$ in two steps.

The 1st step ([6]). Let $L(z)$, $B(z)$ be given by

$$L(z) = i(1-2\Pi(z))\frac{d\Pi(z)}{dz}, \tag{2.15}$$

$$i\frac{dB(z)}{dz} = L(z)B(z); \quad B(0) = 1. \tag{2.16}$$

We refer to Reed and Simon [6] for the proof of the fact that $B(z)$ is analytic and invertible in J_d and satisfies the conditions a. and b. of the Lemma 1.

The 2nd step. Consider $B(2\pi)$. Since

$$B(z)\Pi(0)B^{-1}(z) = \Pi(z), \tag{2.17}$$

it follows from $\Pi(0) = \Pi(2\pi)$ that

$$B(2\pi) = B_1 \oplus B_2, \tag{2.18}$$

where the orthogonal sum is according to the decomposition

$$\mathcal{K} = \Pi(0)\mathcal{K} \oplus (1-\Pi(0))\mathcal{K}. \tag{2.19}$$

Since B_1 and B_2 are unitary operators, one can take the logarithm, i.e., there exist bounded self-adjoint operators C_1, C_2 in $\Pi(0)\mathcal{K}$ and $(1-\Pi(0))\mathcal{K}$, respectively, such that $\|C_i\| \le 1$, $i = 1,2$, and

$$B(2\pi) = \exp(2\pi i C), \quad C = C_1 \oplus C_2. \tag{2.20}$$

Obviously $[C, \Pi(0)] = 0$, and consequently,

$$[\Pi(0), \exp(izC)] = 0. \tag{2.21}$$

We claim now that the family

$$A(z) = B(z)\exp(-izC) \tag{2.22}$$

satisfies all the conditions a–c Lemma 1. Combining (2.17) and (2.22) one obtains the property a. for $A(z)$. Since $B(z)$ is unitary for $z \in R$ [6] and C is self-adjoint, it follows that $A(z)$ is unitary for $z \in R$. Since $B(z)$ is analytic and invertible in J_d, $A(z)$ has the same properties. Finally, using (2.16), the fact that $\Pi(z)$ and $K(z)$ are periodic and (2.21) for $z = 2\pi$, one can easily verify recurrently that

$$\frac{d^n}{dz^n}A(z)\Big|_{z=0} = \frac{d^n}{dz^n}A(z)\Big|_{z=2\pi},$$

which completes the proof.

We are now prepared to prove the following basic Proposition.

Proposition 2. Let $\sigma^\circ(k_1) = \{\lambda_i(k_1)\}_{i=1}^{p}, \sum_{i=1}^{p} r_i = m$ be an isolated band of $H_0(k_1)$, and $P_0(k_1)$ its corresponding spectral projection. Then, there exist a positive constant $d_0>0$ and m valued vector functions $\chi_i^\circ(k_1) \in \mathcal{H}'$, $i = 1,2,\ldots,m$ analytic in the strip J_{d_0}, $\chi_i^\circ(k_1) = \chi_i^\circ(k_1+2\pi)$ such that $\{V^{-1}(k_1)\chi_i^\circ(k_1)\}_1^m$ is an orthonormed basis in $P_0(k_1)\mathcal{H}'$.

Proof. From the fact that $H_0(k_1)$ is an entire function and the fact $\sigma^\circ(k_1)$ is isolated, using the formula

$$P_0(k_1) = \frac{1}{2\pi i}\int_C \frac{1}{H_0(k_1)-z}dz,$$

where C is a contour enclosing $\sigma^\circ(k_1)$, it follows that there exists $d_0 > 0$ (see, e.g., ref. [10]) such that $P_0(k_1)$ is analytic in J_{d_0}. From (2.12) and (2.13) it follows that

$$\Pi_0(k_1) = V(k_1)P_0(k_1)V^{-1}(k_1)$$

is periodic and then satisfies all the conditions of Lemma 1. Let $A(k_1)$ be given by Lemma 1 applied to $\Pi_0(k_1)$ and $\{\chi_i^\circ\}_1^m$ be a basis in $P_0(0)\mathcal{H}'$. Then, from (2.12) and Lemma 1 one can easily see that

$$\chi_i^\circ(k_1) = A(k_1)\chi_i^\circ, \qquad i = 1,2,\ldots,m, \tag{2.23}$$

have all the required properties.

We shall end by writing the position operator $(X_0 f)(\vec{x}) = \vec{n}\vec{x}f(\vec{x})$ for $\vec{n} = (2\pi)^{-1}\vec{K}_1$ in a convenient form. Obviously,

$$(X_0 f)(\vec{x}) = x_1 f(\vec{x}),$$
$$\vec{x} = \sum_{i=1}^{3} x_i \vec{a}_i. \tag{2.24}$$

Consider the Hilbert space $\tilde{\mathcal{H}}$

$$\tilde{\mathcal{H}} = \int_{[0,2\pi]}^{\oplus} \mathcal{H}'dk_1, \tag{2.25}$$

with a self-explanatory notation

$$\mathcal{H} = J \int_{B_\perp}^{\oplus} \tilde{\mathcal{H}}\, d\vec{k}_\perp , \qquad (2.26)$$

J being the Jacobian $J = (|\vec{K}_1||\vec{K}_2||\vec{K}_3|)^{-1} (\vec{K}_1 \cdot (\vec{K}_2 \times \vec{K}_3))$.
We shall denote the elements of $\tilde{\mathcal{H}}$ by $\{\psi_{\vec{m}}(k_1)\}_{\vec{m} \in \mathbf{Z}^3;\, k_1 \in [0,2\pi]}$
Consider the operator $\tilde{X}_0$ given by

$$\{(\tilde{X}_0 \psi)_{\vec{m}}(k_1)\} = \{i \frac{d}{dk_1} \psi_{\vec{m}}(k_1)\} , \qquad (2.27)$$

$$D(\tilde{X}_0) = \{\{\psi_{\vec{m}}(k_1)\} | \{\frac{d}{dk_1} \psi_{\vec{m}}(k_1)\} \in \tilde{\mathcal{H}};\ \psi_{m_1,m_2,m_3}(2\pi) = \psi_{m_1+1,m_2,m_3}(0)\}.$$

Proposition 3. Let X_0 be the self-adjoint operator in $L^2(\mathbf{R}^3, d\vec{x})$

$$(X_0 f)(\vec{x}) = x_1 f(\vec{x}) ; \quad \vec{x} = \sum_{i=1}^{3} x_i \vec{a}_i$$

on its natural domain. Then

$$U X_0 U^{-1} = \int_{B_\perp}^{\oplus} \tilde{X}_0\, d\vec{k}_\perp . \qquad (2.28)$$

The simple proof of this Proposition is left to the reader.

The operator $\tilde{X}_0$ is a self-adjoint extension of $i \frac{d}{dk_1}$ described by somewhat unusual boundary conditions. The next remark is that $\tilde{X}_0$ is related to a more familiar self-adjoint extension of $i \frac{d}{dk_1}$. Let

$$\tilde{V} = \int_{[0,2\pi]}^{\oplus} V(k_1) dk_1 ; \qquad \tilde{M} = \int_{[0,2\pi]}^{\oplus} M\, dk_1 \qquad (2.29)$$

(remember that $V(k_1) = \exp(ik_1 M))$) and $i(\frac{d}{dk_1})_{per}$, the self-adjoint operator, be given by

$$\{(i(\frac{d}{dk_1})_{per.} \psi)_{\vec{m}}(k_1)\} = \{i \frac{d}{dk_1} \psi_{\vec{m}}(k_1)\} ,$$

$$(2.30)$$

$$D(i(\frac{d}{dk_1})_{per.}) = \{\{\psi_{\vec{m}}(k_1)\} | \{\frac{d}{dk} \psi_{\vec{m}}(k_1)\} \in \mathcal{H}';\ \psi_{\vec{m}}(0) = \psi_{\vec{m}}(2\pi)\} .$$

Proposition 4.

$$\tilde{V} \tilde{X}_0 \tilde{V}^{-1} = i(\frac{d}{dk_1})_{per} + \tilde{M} . \qquad (2.31)$$

Proof. This is an immediate consequence of the differentiability of $V(k_1)$ and of the fact that

$$(V(2\pi)\psi)_{m_1,m_2,m_3} = \psi_{m_1-1,m_2,m_3} .$$

Remarks 3.

Proposition 2 asserts the existence of quasi-Bloch functions $\chi_i^{\circ}(k_1)$ (/2,3/) which are analytic and periodic in k_1 at $\vec{k}_\perp$ fixed. This Proposition implies the existence of Wannier functions decreasing exponentially in the $\vec{a}_1$ direction. We would like to stress that Proposition 2 does not imply the exponential degrease of Wannier functions in all directions. In order to prove this, one needs the generalization of Proposition 2, asserting the analyticity and periodicity in all variables k_1, k_2, k_3. This is not a trivial problem, due to some topological difficulties; this problem is beyong the scope of this paper, and will be considered elsewhere.

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Received by Publishing Department
in March 19 1982.

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Аналитичность и периодичность квазиблоховских функций относительно одной переменной

Изучаются некоторые свойства квазиблоховских функций, которые представляют интерес при изучении поведения блоховских электронов во внешнем электрическом поле. Доказывается аналитичность и периодичность квазиблоховских функций относительно одной компоненты квазиимпульса, для общего трехмерного кристалла и вырожденных зон. Метод доказательства основан на одном абстрактном результате, который обобщает метод трансформирующих функций в периодическом случае.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1982

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One Variable Analyticity and Periodicity of the Quasi-Bloch Functions

For general three-dimensional crystals and intersecting bands, the existence of quasi-Bloch functions, analytic and periodic as functions of one of the components of the crystal momentum (the others being fixed) is proved.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Communication of the Joint Institute for Nuclear Research. Dubna 1982