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EXISTENCE OF THE EXPONENTIALLY LOCALISED WANNIER FUNCTIONS

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1. INTRODUCTION

In this paper we shall consider one of the few basic questions of the quantum theory of solids in the one electron approximation which are not yet completely solved: the existence of exponentially localised Wannier functions. We shall consider only nondegenerated bands. For the results obtained so far for degenerated bands we refer to /1,2,3/. Since their appearance /4/ the Wannier functions played a crucial role in developing the theory of slowly varying perturbations in solids. The crucial property of the Wannier functions which makes them so useful is their localisation. From the very definition and the Paley-Wiener theorem it follows at once that the exponential localisation of Wannier functions is equivalent to the analyticity and periodicity of the corresponding Bloch functions as functions of the crystal momentum $\vec{k}$. To our best knowledge all the results concerning the localisation of the Wannier functions are obtained by first proving the existence of Bloch functions analytic and periodic in $\vec{k}$. Our paper is not an exception and all the discussion below as well as the body of the paper is about the existence of analytic and periodic Bloch functions.

The one-dimensional crystals with a center of inversion have been treated in a definitive manner by Kohn in a classic paper /5/. Concerning three-dimensional crystals there is a widespread opinion /12/ that the exponential localisation of the Wannier functions has been proved by Blount /6/. Unfortunately this is not true, because a crucial point is missed in Blount's argument. More exactly through his paper he tacitly assumed that the Bloch functions are periodic in $\vec{k}$. At the same time he proved the analyticity in $\vec{k}$ of the Bloch functions by the $\vec{k}\vec{p}$ perturbation theory: the eigenvalue problem for the periodic part of the Bloch functions is assumed to be solved at a fixed value $\vec{k}_0$ of $\vec{k}_0$; then by the $\vec{k}\vec{p}$ perturbation theory /12/ one obtains the periodic part of the Bloch functions in a neighbourhood of $\vec{k}_0$ as an analytic function of $\vec{k}$: fix $\vec{k}_1$ in this neighbourhood, apply again the $\vec{k}\vec{p}$ perturbation theory, and so on. But the Bloch functions thus obtained may not be periodic (the translation symmetry implies $\vec{k}$ periodicity of the Bloch functions only up to a phase factor). The three dimensional crystals have been considered by des Cloizeaux /1,2/. His method of building analytic and periodic in $\vec{k}$ Bloch functions consists of two steps: i. the proof that the corresponding spectral projection (in which the arbitrary phase factor up to which the eigenvalue problem determines the Bloch functions cancels out) is analytic and periodic in $\vec{k}$; ii. analytic and periodic Bloch functions are constructed, in some way, with the help of the corresponding spectral projection. The first step can be carried out in the general case: many-dimensional crystals and degenerated bands [1] (see also Section 2 below). The second step is the hard one (although at first sight it looks almost trivial[7]) and by his method of trial Wannier functions, des Cloizeaux succeeded to build analytic and periodic Bloch functions only if the (three-dimensional) crystal has a center of inversion[2]. He was also able to treat general one-dimensional crystals but in this case the result is weaker: the domain of analyticity of the Bloch functions may be smaller than that of the corresponding spectral projections.

In this paper the condition of the existence of a centre of inversion is removed. We shall follow the route of des Cloizeaux. In Section 2 up to date presentation of the results concerning the spectral projections corresponding to isolated bands (degenerated or not) is given. In Section 3 we shall prove some abstract results (which might be interesting in themselves) concerning analytic families of projections in Hilbert spaces. In Section 4 using the results in Section 3 we shall prove the existence of analytic and periodic in $\vec{k}$ Bloch functions corresponding to nondegenerated bands in arbitrary (i.e., not necessary with a centre of inversion) crystals of arbitrary dimensionality. Our results are optimal in the sense that the analyticity domain of the Bloch functions coincides with that of the corresponding spectral projections.

2. PRELIMINARIES

In this section we shall recall, in a suitable form, some general properties of the Hamiltonian

$$H = -\Delta + V(\vec{x}), \tag{2.1}$$

where $V(\vec{x})$ is a periodic function. Let $\{\vec{a}_i\}$ be a basis in $\mathbb{R}^3$ and $\{\vec{K}_i\}_{i=1}^3$, be its dual basis, i.e.,

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

Let Q and B be the basic period cells for the basis $\{\vec{a}_i\}$ and $\{\vec{K}_i\}$, respectively.

Theorem 2.1 [8]

Let $V(\vec{x})$ be a real function on $\mathbb{R}^3$ with $V(\vec{x}+\vec{a}_i) = V(\vec{x})$, $i=1,2,3$. Let

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

and

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

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

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

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

$$(H(\vec{k})\psi)_{\vec{m}} = (\vec{k} + \sum_{j=1}^3 m_j \vec{K}_j)^2 \psi_{\vec{m}} + \sum_{\vec{n} \in \mathbf{Z}^3} \hat{V}_{\vec{n}} \psi_{\vec{m}-\vec{n}} \tag{2.2}$$

with the domain

$$\mathcal{D}(H(\vec{k})) = \mathcal{D}_0 = \{\psi \in \mathcal{H}' \mid \sum_{\vec{m} \in \mathbf{Z}^3} |\vec{m}|^2 |\psi_{\vec{m}}|^2 < \infty\} .$$

Then

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

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

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

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

$$(Uf)_{\vec{m}}(\vec{k}) = \hat{f}(\vec{k} + \sum_{j=1}^3 m_j \vec{K}_j); \quad \vec{k} \in B, \tag{2.3}$$

where $\hat{f}$ denotes the Fourier transform of f.

Then U is unitary and

$$UHU^{-1} = \int_B^{\oplus} H(\vec{k}) d\vec{k} . \tag{2.4}$$

Proof. See ref.[8] Chapter XIII.

In what follows, k_i, $i = 1,2,3$ denote the coordinates of $\vec{k}$ with respect to the basis $|\vec{K}_i|^{-1}\vec{K}_i$ and $\vec{K}$ denotes a vector of reciprocical lattice,

$$\Gamma = \{ \vec{K} \mid \vec{K} = \sum_{j=1}^{3} p_j \vec{K}_j \,, \quad p_j \in \mathbf{Z} \}.$$

Let $W_i : \mathcal{H}' \to \mathcal{H}'$, $i = 1,2,3$ be the unitary operators given by

$$(W_1 \psi)_{\vec{m}} = \psi_{m_1 - 1, m_2 m_3} \;; \quad (W_2 \psi)_{\vec{m}} = \psi_{m_1, m_2 - 1, m_3} \;; \quad (W_3 \psi)_{\vec{m}} = \psi_{m_1, m_2, m_3 - 1} \tag{2.5}$$

Since W_i are unitary and 1 is not an eigenvalue of W_i, there exist unique self-adjoint operators M_i such that $\| M_i \| \le 2\pi / |\vec{K}_i|$ and

$$W_i = \exp(i |\vec{K}_i| M_i) . \tag{2.6}$$

Consider now the bounded operator valued function

$$W(\vec{k}) = \exp(i \sum_{j=1}^{3} k_j M_j) = \prod_{j=1}^{3} \exp(i k_j M_j), \quad \vec{k} \in \mathbf{C}^3 \tag{2.7}$$

(remark that M_i commute). Obviously $W(\vec{k})$ is an entire function of three complex variables and moreover

$$W^*(\vec{k}) = W^{-1}(\vec{k}), \qquad \vec{k} \in \mathbf{R}^3 . \tag{2.8}$$

Lemma 2.1.[3] Let $L(\vec{k})$ be given by

$$L(\vec{k}) = W(\vec{k}) H(\vec{k}) W^{-1}(\vec{k}) \tag{2.9}$$

Then for all $\vec{K} \in \Gamma$ and $\vec{k} \in \mathbf{C}^3$

$$L(\vec{k}) = L(\vec{k} + \vec{K}). \tag{2.10}$$

Proof. The proof is a straightforward, although a little bit tedious verification.

Let $\sigma(\vec{k})$ be the (discrete by Theorem 2.1 iii) spectrum of $H(\vec{k})$.

Corollary 2.1. As a set

$$\sigma(\vec{k}) = \sigma(\vec{k} + \vec{K}). \tag{2.11}$$

A nonvoid part $\sigma^{\circ}(\vec{k})$ of $\sigma(\vec{k})$, $\vec{k} \in B \subset \mathbf{R}^3$ is said to be an isolated band of $H(\vec{k})$ if there exist continuous and periodic functions $f_i(\vec{k}) : \mathbf{R}^3 \to \mathbf{R}$ $f_i(\vec{k}) = f_i(\vec{k} + \vec{K})$ $i = 1,2$ and a positive constant $c > 0$ such that $f_1(\vec{k}) < f_2(\vec{k})$ and

$$\sigma^{\circ}(\vec{k}) \subset [f_1(\vec{k}), f_2(\vec{k})] ,$$

$$\sigma(\vec{k}) \cap [f_i(\vec{k}) - c ,\; f_i(\vec{k}) + c] = \phi \qquad i = 1,2 .$$

Let $P_0(\vec{k})$, $\vec{k} \in \mathbf{R}^3$ be the spectral projection of $H(\vec{k})$ corresponding to an isolated band $\sigma^{\circ}(\vec{k})$.

Lemma 2.2.[7,8] There exist $a > 0$, $D \subset \mathbf{R}^3$, $D \supset \{ \vec{y} \in \mathbf{R}^3 \mid |\vec{y}| \le a \}$ such that $P_0(\vec{k})$ is the restriction to $\mathbf{R}^3$ of a bounded projection valued function analytic in

$$\mathcal{I}_D^3 = \{ \vec{z} = \vec{x} + i\vec{y} \in \mathbf{C}^3 \mid \vec{x} \in \mathbf{R}^3, \; \vec{y} \in D \}.$$

Proof. This is a direct consequence of the theory of analytic perturbations as developed in ref.[8].

From Lemma 2.2 it follows, in particular, that $\dim P_0(\vec{k})$ is constant and due to Theorem 2.1 iii, finite. An isolated band $\sigma^{\circ}(\vec{k})$ is said to be nondegenerated of $P_0(\vec{k}) = 1$.

Consider the following (antiunitary) involution $\theta : \mathcal{H}' \to \mathcal{H}'$

$$(\theta \psi)_{\vec{m}} = \bar{\psi}_{-\vec{m}} . \tag{2.12}$$

Lemma 2.3. For $\vec{k} \in \mathbf{R}^3$

$$\theta P_0(\vec{k}) \theta = P_0(-\vec{k}) , \tag{2.13}$$

$$\theta W(\vec{k}) \theta = W(-\vec{k}). \tag{2.14}$$

Proof. From the reality of $V(\vec{x})$, (2.2) and the definition of θ it follows that for $\vec{k} \in \mathbf{R}^3$

$$\theta H(\vec{k}) \theta = H(-\vec{k})$$

which implies (2.13) via the formula relating $P_0(\vec{k})$ and the resolvent of $H(\vec{k})$. From (2.5) and (2.12) it follows that

$$\theta W_i \theta = W_i^{-1} = W_i^* = \exp(-i |\vec{K}_i| M_i). \tag{2.15}$$

On the other hand,

$$\theta \; W_i \; \theta = \theta \exp(i |\vec{K}_i| M_i) \theta = \exp(-i |\vec{K}_i| \theta M_i \theta). \tag{2.16}$$

Combining (2.15), (2.16) and using the uniqueness of M_i one obtains

$$\theta M_i \theta = M_i \tag{2.17}$$

thereof (2.14) follows.

We shall summarize the above results in the following (see also ref.[1]).

Theorem 2.2. Let $\sigma^\circ(\vec{k})$ be an isolated band of $H(\vec{k})$, $P_0(\vec{k})$ be the spectral projection of $H(\vec{k})$ corresponding to $\sigma^\circ(\vec{k})$ and $Q(\vec{k})$ defined by

$$Q(\vec{k}) = W(\vec{k})P_0(\vec{k})W^{-1}(\vec{k}), \quad \vec{k} \in R^3 . \tag{2.18}$$

Then $Q(\vec{k})$ is the restriction to R^3 of a bounded projection valued function analytic in $\mathcal{J}^3_D$ and satisfying

$$Q(\vec{k}) = Q(\vec{k}+\vec{K}), \quad \vec{k} \in \mathcal{J}^3_D, \quad \vec{K} \in \Gamma , \tag{2.19}$$

$$\theta Q(\vec{k})\theta = Q(-\vec{k}), \quad \vec{k} \in R^3 . \tag{2.20}$$

3. ANALYTIC FAMILIES OF PROJECTIONS IN HILBERT SPACES

In what follows $\vec{z}^j = (z_1,...,z_j) \in C^j$, $\vec{p}^j = (p_1,...,p_j) \in Z^j$. In this section we shall discuss the following two problems.

Problem A.

Let $\mathcal{K}$ be a separable Hilbert space, q be a positive integer, $\mathcal{J}^q_a = \{\vec{z}^q \in C^q \,|\, |\mathrm{Im}\, z_i| < a,\ a > 0\}$ and $Q(\vec{z}^q)$ be a projection valued function analytic in $\mathcal{J}^q_a$ and satisfying

$$Q(\vec{z}^q) = Q^*(\vec{z}^q), \quad \vec{z}^q \in R^q . \tag{3.1}$$

Find a bounded with bounded inverse operator valued function $A(\vec{z}^q)$ analytic in $\mathcal{J}^q_a$ satisfying

$$A(\vec{z}^q)Q(0) = Q(\vec{z}^q)A(\vec{z}^q), \quad A(0) = 1, \tag{3.2}$$

$$A^*(\vec{z}^q) = A^{-1}(\vec{z}^q), \quad \vec{z}^q \in R^q . \tag{3.3}$$

Problem B.

Under the conditions of Problem A, suppose in addition that $Q(\vec{z}^q)$ is periodic, i.e., for arbitrary $\vec{p}^q \in Z^q$

$$Q(\vec{z}^q) = Q(\vec{z}^q + 2\pi\vec{p}^q), \quad \vec{z}^q \in \mathcal{J}^q_a . \tag{3.4}$$

Find $A(\vec{z}^q)$ satisfying beside the requirements of Problem A

$$A(\vec{z}^q)Q(0) = A(\vec{z}^q + 2\pi\vec{p}^2)Q(0), \quad \vec{z}^q \in \mathcal{J}^q_a, \vec{p}^q \in Z^q . \tag{3.5}$$

To our best knowledge, up to now only Problem A for $q = 1$ (but in a more general setting: arbitrary simply connected domains, Banach spaces, etc.) has been thoroughly investigated[8,9] (see, however,[3,10] where Problem B for $q = 1$ is discussed). There are (at least two methods of constructing solutions of Problems A and B. The first one (in a slightly different form going back to Sz-Nagy[9]) is based on the following result concerning the unitary equivalence of pairs of orthogonal projections in Hilbert spaces.

Lemma 3.1.[9]

Let Q_1, Q_2 be self-adjoint projections in $\mathcal{K}$ satisfying

$$\|Q_1 - Q_2\| < 1. \tag{3.6}$$

Then the operator

$$A_{2,1} = (1-(Q_1-Q_2)^2)^{-1/2}(Q_2Q_1 + (1-Q_2)(1-Q_1)) \tag{3.7}$$

is unitary and

$$A_{2,1}Q_1A^{-1}_{2,1} = Q_2. \tag{3.8}$$

Proof. See[9] II 4.6.

The above lemma gives at once.

Proposition 3.1. Suppose

$$\|Q(\vec{z}^q) - Q(0)\| < 1 \quad \text{for } \vec{z}^q \in \mathcal{J}^q_a . \tag{3.9}$$

Then

$$A(\vec{z}^q) = (1-(Q(\vec{z}^q) - Q(0))^2)^{-1/2}$$

$$(Q(\vec{z}^{\,q})Q(0) + (1-Q(\vec{z}^{\,q}))(1-Q(0))) \tag{3.10}$$

is a solution of Problems A and B.

Proof. The proof of (3.8) does not depend on the self-adjointness of Q_1 and Q_2. Unfortunately the condition (3.9) is a very restrictive one (see [9] Remark 4.4 in Chap.II). One can generalize (3.10) to give a solution of Problem A.

Proposition 3.2. Let $0<R<\infty$, $0<b<a$. Then there exists a positive integer N depending on R and b such that

$$A_N(\vec{z}^{\,q}) = \prod_{\ell=0}^{N-1} [(1-(Q(\tfrac{N-\ell}{N}\vec{z}^{\,q}) - Q(\tfrac{N-\ell-1}{N}\vec{z}^{\,q}))^2)^{-1/2}$$

$$\times (Q(\tfrac{N-\ell}{N}\vec{z}^{\,q})Q(\tfrac{N-\ell-1}{N}\vec{z}^{\,q}) + (1-Q(\tfrac{N-\ell}{N}\vec{z}^{\,q}))(1-Q(\tfrac{N-\ell-1}{N}\vec{z}^{\,q})))] \tag{3.11}$$

is a solution of Problem A for $\vec{z}^{\,q} \in \{\vec{z}^{\,q} \in \mathbf{C}^q \mid |\mathrm{Re}\, z_i| < R, |\mathrm{Im}\, z_i| < b, i = 1,\ldots,q\}$.

Proof. This is a simple iteration of Proposition 3.1. Clearly (3.11) is not suitable for solving Problem B since $A_N(\vec{z}^{\,q})$ has no required periodicity properties for $N>1$.

The second method of constructing solutions of Problem A has been put forward independently by Daletsky and Krein and Kato (see references in[8,11]). The basic construction is contained in

Lemma 3.2.[9] Let $Q(t)$, $t \in \mathbf{R}$ be a norm differentiable family of bounded projections with norm continuous derivative and $A(t)$ be given as unique solution of the equation

$$i\frac{d}{dt}A(t) = i((1-2Q(t))\frac{d}{dt}Q(t))A(t), \quad A(0) = 1. \tag{3.12}$$

Then

i.

$$A(t)Q(0) = Q(t)A(t), \quad t \in \mathbf{R}. \tag{3.13}$$

ii. If $Q(t)$ is self-adjoint then $A(t)$ is unitary.

Proof. See[8,9,11].

The above lemma gives at once a solution of Problem A for $q=1$ (also the generalization to $q>1$ is straightforward). As it stands, the above lemma does not give solutions of Problem B (see ref.[9] Remark 4.2 Chap.II). However, Lemma 3.2 combined with some results in the theory of differential equations with periodic coefficients allows a construction of $A(z)$ solving Problem B for $q=1$ (see also[10] for finite dimensional $\mathcal{K}$).

Proposition 3.3.[3] For $q=1$ Problem B admits solutions.

Proof. See[3].

Summarizing the above discussion, Problem A for all $q=1,2,\ldots$ and Problem B for $q=1$ admit solutions without any additional conditions on $Q(\vec{z}^{\,q})$. In contrast, it seems very probable that for $q>1$, in general Problem B does not admit solutions. One sufficient condition for Problem B to have a solution is provided by Proposition 3.1. Unfortunately (3.9) is a severe restriction on the variation of $Q(\vec{z}^{\,q})$ and the result in Proposition 3.1 seems not to be very interesting for applications (e.g., concerning the localization of Wannier functions it covers only the tight binding limit). Motivated by the concrete problem at hand, the main new result of this section gives another example of sufficient conditions for the existence of a solution to Problem B.

Theorem 3.1. Under the conditions of Problem B suppose:

i.

$$\dim Q(\vec{z}^{\,q}) = 1 \tag{3.14}$$

ii. There exists an antilinear involution $\theta: \mathcal{K} \to \mathcal{K}$ such that

$$\theta Q(\vec{z}^{\,q})\theta = Q(-\vec{z}^{\,q}), \quad \vec{z}^{\,q} \in \mathbf{R}^q. \tag{3.15}$$

Then $A(\vec{z}^{\,q})$ satisfying the requirements of Problem B exists.

Proof. The proof is by construction and consists of two steps. At the first step, using Lemma 3.2 we shall construct $B(\vec{z}^{\,q})$ satisfying (3.2-4) but not (3.5). At the second step we shall "correct" the construction of the first step as to provide $A(\vec{z}^{\,q})$ satisfying all the requirements of the theorem. It is the second step where we shall use crucially the conditions (3.14) and (3.15). During the proof, some of the technical points are states as lemmas which are proved at the end. The main point of the proof is Lemma 3.3 below.

Step 1. Fix $z_1, \ldots, z_{q-1}$ and let $B_q(\vec{z}^q)$ be given as a solution of the differential equation

$$i \frac{d}{dz_q} B_q(\vec{z}^q) = i((1-2Q(\vec{z}^q)) \frac{d}{dz_q} Q(\vec{z}^q)) B_q(\vec{z}^q), \tag{3.16}$$

$$B_q(\vec{z}^{q-1}, 0) = 1.$$

Lemma 3.2 and standard results about analyticity properties of the solutions of differential equations in terms of the analyticity properties of the coefficients imply /8/,/9 II §4/ that $B_q(\vec{z}^q)$ is analytic in $\mathcal{J}_a^q$, has bounded inverse and

$$B^*_q(\vec{z}^q) = B_q^{-1}(\vec{z}^q), \quad \vec{z}^q \in R^q. \tag{3.17}$$

$$B_q(\vec{z}^q) Q(\vec{z}^{q-1}, 0) = Q(\vec{z}^q) B_q(\vec{z}^q), \quad \vec{z}^q \in \mathcal{J}_a^q. \tag{3.18}$$

One can repeat the same procedure starting from $Q(z^{q-1}, 0)$ and construct $B_{q-1}(\vec{z}^{q-1})$. After q steps one obtains $B(\vec{z}^q)$ in the form

$$B(\vec{z}^q) = B_q(\vec{z}^q) B_{q-1}(\vec{z}^{q-1}) \ldots B_1(z_1) \tag{3.19}$$

which satisfies (3.2) and (3.3).

Step 2. Consider

$$T(\vec{z}^{q-1}) = B_q(\vec{z}^{q-1}, \pi) B_q^{-1}(\vec{z}^{q-1}, -\pi). \tag{3.20}$$

From (3.2), (3.4) and (3.20) it follows that

$$[T(\vec{z}^{q-1}), Q(\vec{z}^{q-1}, \pi)] = 0. \tag{3.21}$$

This implies that with respect to the direct sum decomposition

$$K = Q(\vec{z}^{q-1}, \pi) K \dot{+} (1-Q(\vec{z}^{q-1}, \pi))K \tag{3.22}$$

$T(\vec{z}^{q-1})$ takes a direct sum form

$$T(\vec{z}^{q-1}) = T_1(\vec{z}^{q-1}) \dot{+} T_2(\vec{z}^{q-1}). \tag{3.23}$$

It follows (remember that $\dim Q(\vec{z}^q) = 1$) that if $f \in K$ is decomposed according to (3.22)

$$f = f_1(\vec{z}^{q-1}) \dot{+} f_2(\vec{z}^{q-1})$$

then

$$T(\vec{z}^{q-1}) f = \lambda(\vec{z}^{q-1}) f_1(\vec{z}^{q-1}) \dot{+} (T_2 f_2)(\vec{z}^{q-1}), \tag{3.24}$$

where $\lambda(\vec{z}^{q-1})$ is a complex-valued function.

Lemma 3.3. There exists a unique function $\phi(\vec{z}^{q-1})$ analytic in $\mathcal{J}_a^{q-1}$, with the properties

$$\lambda(\vec{z}^{q-1}) = \exp(2\pi i \phi(\vec{z}^{q-1})), \tag{3.25}$$

$$\phi(0) \in [0, 2\pi), \tag{3.26}$$

$$\phi(\vec{z}^{q-1}) = \overline{\phi(\vec{z}^{q-1})}, \quad \vec{z}^{q-1} \in R^{q-1}, \tag{3.27}$$

$$\phi(\vec{z}^{q-1} + 2\pi \vec{p}^{q-1}) = \phi(\vec{z}^{q-1}), \quad \vec{p}^{q-1} \in Z^{q-1}, \vec{z}^{q-1} \in \mathcal{J}_a^{q-1}. \tag{3.28}$$

Consider

$$A_q(\vec{z}^q) = \exp(-i z_q \phi(\vec{z}^{q-1})) B_q(\vec{z}^q). \tag{3.29}$$

By construction $A_q(\vec{z}^q)$ is analytic in $\mathcal{J}_a^q$, has a bounded inverse, is unitary for $\vec{z}^q \in R^q$, $A_q(0) = 1$ and

$$A_q(\vec{z}^q) Q(\vec{z}^{q-1}, 0) = Q(\vec{z}^q) A_q(\vec{z}^q). \tag{3.30}$$

The periodicity properties of $A_q(\vec{z}^q)$ are given in the following

Lemma 3.4. For $\vec{z}^q \in \mathcal{J}_a^q$ and $\vec{p}^q \in Z^q$

$$A_q(\vec{z}^q) Q(\vec{z}^{q-1}, 0) = A_q(\vec{z}^q + 2\pi \vec{p}^q) Q(\vec{z}^{q-1}, 0). \tag{3.31}$$

In a similar way "correcting" $B_\ell(\vec{z}^\ell)$ one can construct the corresponding $A_\ell(\vec{z}^\ell)$. Then one can verify that

$$A(\vec{z}^q) = A_q(\vec{z}^q) \ldots A_1(z_1) \tag{3.32}$$

satisfies all the requirements of the theorem. Let us verify for example (3.5) for $q = 2$

$$A_2(\vec{z}^2) A_1(z_1) Q(0) = A_2(\vec{z}^2) Q(z_1, 0) A_1(z_1) Q(0) =$$

$$= A_2(\vec{z}^2 + 2\pi \vec{p}^2) Q(z_1, 0) A_1(z_1 + 2\pi p_1) Q(0) =$$

$$= A_2(\vec{z}^2 + 2\pi \vec{p}^2) Q(z_1 + 2\pi p_1, 0) A_1(z_1 + 2\pi p_1) Q(0)$$

$$= A(\vec{z}^{\,2} + 2\pi\vec{p}^{\,2}) A_1(z_1 + 2\pi p_1) Q(0). \tag{3.33}$$

The proof of Theorem 3.1 is completed.

Proof of Lemma 3.3. The invertibility of $T(\vec{z}^{\,q-1})$ and (3.24) imply that $\lambda(\vec{z}^{\,q-1}) \neq 0$ for $\vec{z}^{\,q-1} \in \mathcal{J}_a^{q-1}$. Let now $f \in Q(\vec{0}^{\,q-1}, \pi)\mathcal{K}$. There exists a neighbourhood X of 0 in $\mathbf{C}^{q-1}$ such that $(f, Q(\vec{z}^{\,q-1}, \pi) f) \neq 0$. Then from (3.24) it follows that

$$\lambda(\vec{z}^{\,q-1}) = (f, Q(\vec{z}^{\,q-1}, \pi) f)^{-1} (f, Q(\vec{z}^{\,q-1}, \pi) T(\vec{z}^{\,q-1}) f) \tag{3.34}$$

wherefrom $\lambda(\vec{z}^{\,q-1})$ is analytic in X. By an analytic continuation argument $\lambda(\vec{z}^{\,q-1})$ is analytic in $\mathcal{J}_a^{q-1}$. It follows that (3.25) is true with $\phi(\vec{z}^{\,q-1})$ analytic in $\mathcal{J}_a^{q-1}$. The function $\phi(\vec{z}^{\,q-1})$ is uniquely fixed by its value at zero. For $\vec{z}^{\,q-1} \in \mathbf{R}^{q-1}$, $T(\vec{z}^{\,q-1})$ is unitary and the decomposition (3.22) is an orthogonal one which proves (3.26). From (3.16) and (3.4) it follows that $B_q(\vec{z}^{\,q})$ is periodic in $\vec{z}^{\,q-1}$ which implies the periodicity of $\lambda(\vec{z}^{\,q-1})$. Since $\frac{d\lambda}{dz_i} = i\lambda \frac{d\phi}{dz_i}$, $\frac{d\phi}{dz_i}$ are periodic whereof it follows that

$$\phi(\vec{z}^{\,q-1}) = \psi(\vec{z}^{\,q-1}) + \sum_{\ell=1}^{q-1} p_\ell z_\ell , \tag{3.35}$$

where ψ is periodic and p_ℓ are integers. We shall prove now that (3.15) implies

$$\phi(\vec{z}^{\,q-1}) = \phi(-\vec{z}^{\,q-1}). \tag{3.36}$$

From (3.15) and (3.16) it follows

$$i \frac{d}{dz_q} \theta B_q(-\vec{z}^{\,q}) \theta = i((1 - 2Q(\vec{z}^{\,q})) \frac{d}{dz_q} Q(\vec{z}^{\,q})) \theta B_q(-\vec{z}^{\,q}) \theta \tag{3.37}$$

whereof

$$\theta B_q(-\vec{z}^{\,q}) \theta = B_q(\vec{z}^{\,q}). \tag{3.38}$$

Taking into account (3.38) and the definition of T one obtains

$$\theta T(-\vec{z}^{\,q-1}) \theta = T^{-1}(\vec{z}^{\,q-1}), \quad \vec{z}^{\,q-1} \in \mathbf{R}^{q-1} . \tag{3.39}$$

From (3.15) and (3.4) one has

$$\theta Q(\vec{z}^{\,q-1}, \pi) \theta = Q(-\vec{z}^{\,q-1}, \pi). \tag{3.40}$$

Let now $f \in Q(-\vec{z}^{\,q-1}, \pi)\mathcal{K}$. Then using (3.27), (3.39) and (3.40)

$$\begin{aligned} \theta T(\vec{z}^{\,q-1}) \theta f &= \exp(-2\pi i \phi(-\vec{z}^{\,q-1})) f = \\ &= \exp(-2\pi i \phi(\vec{z}^{\,q-1})) f , \quad \vec{z}^{\,q-1} \in \mathbf{R}^{q-1} \end{aligned} \tag{3.41}$$

which proves (3.36). Now (3.36) implies $p_\ell = 0$ in (3.35). Indeed, for example $\phi(-\pi, 0, \dots, 0) = \psi(-\pi, 0, \dots, 0) - p_1\pi = \psi(\pi, 0, \dots, 0) + \pi p_1$ which together with the periodicity of ψ implies $p_1 = 0$. Since the periodicity for $\vec{z}^{\,q-1} \in \mathbf{R}^{q-1}$ and the analyticity in $\mathcal{J}_a^{q-1}$ implies the periodicity in $\mathcal{J}_a^{q-1}$ the proof of Lemma 3.3 is completed.

Proof of Lemma 3.4. From (3.16) and (3.27) it follows

$$\begin{aligned} & i \frac{d}{dz_q} A_q(\vec{z}^{\,q}) Q(\vec{z}^{\,q-1}, 0) = \\ & [i(1 - 2Q(\vec{z}^{\,q})) \frac{d}{dz_q} Q(\vec{z}^{\,q}) + \phi(\vec{z}^{\,q-1})] A_q(\vec{z}^{\,q}) Q(\vec{z}^{\,q-1}, 0), \\ & A_q(\vec{z}^{\,q-1}, 0) Q(\vec{z}^{\,q-1}, 0) = Q(\vec{z}^{\,q-1}, 0). \end{aligned} \tag{3.42}$$

The periodicity in $\vec{z}^{\,q-1}$ is obvious. For periodicity in z_q the only thing we have to verify is that

$$A_q(\vec{z}^{\,q-1}, -\pi) Q(\vec{z}^{\,q-1}, 0) = A_q(\vec{z}^{\,q-1}, \pi) Q(\vec{z}^{\,q-1}, 0). \tag{3.43}$$

Using (3.4), (3.18), (3.20), (3.32), (3.23) and the definition of A_q it follows:

$$\begin{aligned} & A_q(\vec{z}^{\,q-1}, -\pi) Q(\vec{z}^{\,q-1}, 0) = \\ & = \exp(i\pi\phi(\vec{z}^{\,q-1})) T^{-1}(\vec{z}^{\,q-1}) B_q(\vec{z}^{\,q-1}, \pi) Q(\vec{z}^{\,q-1}, 0) = \\ & = \exp(i\pi\phi(\vec{z}^{\,q-1})) T^{-1}(\vec{z}^{\,q-1}) Q(\vec{z}^{\,q-1}, \pi) B_q(\vec{z}^{\,q-1}, \pi) = \\ & = \exp(-i\pi\phi(\vec{z}^{\,q-1})) B_q(\vec{z}^{\,q-1}, \pi) Q(\vec{z}^{\,q-1}, 0) = \\ & = A_q(\vec{z}^{\,q-1}, \pi) Q(\vec{z}^{\,q-1}, 0) \end{aligned}$$

and the proof of Lemma 3.4 is completed.

4. THE WANNIER FUNCTIONS

Applying Theorem 3.1 to the situation described in Theorem 2.2, one obtains

Theorem 4.1. Let $\sigma^{\circ}(\vec{k})$, $\vec{k} \in R^3$ be an isolated band of $H(\vec{k})$, $P_0(\vec{k})$ be the spectral projection of $H(\vec{k})$ corresponding to $\sigma^{\circ}(\vec{k})$, $\dim P_0(\vec{k}) = 1$. Then there exists a vector valued function $\chi^{\circ}(\vec{k})$ analytic in $\mathcal{J}^3_D$ and satisfying

$$W(\vec{k})\chi^{\circ}(\vec{k}) = W(\vec{k}+\vec{K})\chi^{\circ}(\vec{k}+\vec{K}), \quad \vec{k} \in \mathcal{J}^3_D, \quad \vec{K} \in \Gamma, \tag{4.1}$$

$$\chi^{\circ}(\vec{k}) \in P_0(\vec{k})\mathcal{H}, \quad \|\chi^{\circ}(\vec{k})\| = 1, \quad \vec{k} \in R^3. \tag{4.2}$$

Proof. Let us first remark that although Theorem 3.1 has been proved for $\mathcal{J}^3_a$, the proof goes through without changes for $\mathcal{J}^3_D$. Let $A(\vec{k})$ be the operator valued function given by Theorem 3.1 applied to $W(\vec{k})P_0(\vec{k})W^{-1}(\vec{k})$ and $\chi^{\circ} \in P_0(0)\mathcal{H}$, $\|\chi^{\circ}\| = 1$. Then $\chi^{\circ}(\vec{k}) = W^{-1}(\vec{k})A(\vec{k})\chi^{\circ}$ satisfies (4.1) and (4.2).

Corollary 4.1. Let

$$w = (\mathrm{vol}\,Q)^{-1} \int_B^{\oplus} \chi^{\circ}(\vec{k})\,d\vec{k} \qquad \vec{a} \in D, \quad a_i > 0. \tag{4.3}$$

Then

$$\exp\Big(\sum_{j=1}^{3} 2\pi |K_j|^{-1} a_j |\vec{x}_j|\Big)(U^{-1}w)(\vec{x}) \in L^2(R^3), \tag{4.4}$$

where x_i are coordinates of $\vec{x}$ with respect to the basis $\{\vec{a}_i\}$.

Proof. From the definition of $W(\vec{k})$ and Theorem 4.1 it follows that $\widehat{(U^{-1}w)}(\vec{p})$ is the restriction to R^3 of an analytic function in $\mathcal{J}^3_D$. Moreover

$$\int_{R^3} |\widehat{(U^{-1}w)}(\vec{p}+i\vec{a})|^2\,d\vec{p} < \infty .$$

Now (4.4) follows from the Paley-Wiener theorem.

The Wannier functions corresponding to $\sigma^{\circ}(\vec{k})$ are defined as follows[12]

$$w^{\circ}_{\nu}(\vec{x}) = w^{\circ}\Big(\vec{x} - \sum_{j=1}^{3} \nu_j \vec{a}_j\Big), \qquad \nu_j - \text{integers}$$
$$w^{\circ}(\vec{x}) = (\mathrm{vol}\,Q)^{-1} \int_B \psi_{o,\vec{k}}(\vec{x})\,d\vec{k}, \tag{4.5}$$

where $\psi_{o,\vec{k}}(\vec{x}) = \exp(i\vec{k}\vec{x})u_{o,\vec{k}}(\vec{x})$ are Bloch functions corresponding to $\sigma^{\circ}(\vec{k})$. Looking at the equation satisfied by the periodic part $u_{o,\vec{k}}(\vec{x})$ of $\psi_{o,\vec{k}}(\vec{x})$ one gets that $u_{o,\vec{k}}(\vec{x})$ is nothing but the "$\vec{x}$-representation" of $\chi^{\circ}(\vec{k})$. Comparing (4.3) with (4.5) one finds that

$$w^{\circ}(\vec{x}) = (U^{-1}w)(\vec{x})$$

which together with Corollary 4.1 gives:

Theorem 4.2. There exist Wannier functions corresponding to an isolated nondegenerated band of H which are exponentially localised.

REFERENCES

1. Des Cloizeaux J. Phys.Rev., 1964, 135A, p.685-697.
2. Des Cloizeaux J. Phys.Rev., 1964, 135A, p.698-707.
3. Nenciu A., Nenciu G. Dynamics of Bloch Electrons in External Electric Fields. II. The Existence of Stark-Wannier Ladder Resonances. J.Phys.A (to appear).
4. Wannier G.H. Phys.Rev., 1937, 52, p.191-193.
5. Kohn W. Phys.Rev., 1958, 115, p.809-821.
6. Blount I.E. Solid State Physics, 1962, 13, p.305-373.
7. Bentosela F. Comm.Math.Phys., 1979, 68, p.173-182.
8. Reed M., Simon B. Methods of Modern Mathematical Physics. Academic Press, New York, San Francisco, London, 1978, vol.4.
9. Kato T. Perturbation Theory of Linear Operators. Springer, Berlin, Heidelberg, New York, 1966.
10. Sibuya Y. Math.Ann., 1965, 161, p.67-77.
11. Krein S.G. Linear Differential Equations in Banach Spaces. "Nauka". Moscow, 1967.
12. Callaway J. Quantum Theory of the Solid State. Academic Press, New York, 1974.

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